A Computational Approach to Statistics

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Preface

Goal

The purpose of this book is to provide an introduction to statistics with an emphasis on appropriate methods of computation with modern algorithms. We hope it will provide a useful introductory reference for persons with a need to analyze data using computers.

Program listings are included in the appendices so that modifications and corrections can be made as desired. Suggestions, corrections, and errors will be appreciatively received at the e-mail address **Klotz@stat.wisc.edu**.

Organization

Topics covered are as follows, namely:

(1) Descriptive Statistics.

(2) Discrete Probability.

(3) Random Variables

(4) Continuous Probability.

(5) The General Measure Theory Model

(6) Distribution Measures

(7) Multivariate Distributions.

(8) Characteristic Functions

(9) Asymptotics

(10) Sampling Theory for Statistics.

(11) Point Estimatiom.

(12) Hypothesis Testing.

(13) Interval Estimation.

(14) The General Linear Hypothesis.

(15) Nonparametric Methods.

Ends of proofs are labeled with ■ .

Contents

List of Figures

List of Tables

Chapter 1

Descriptive Statistics

1.1 Graphic Description of Data

1.1.1 Histograms

Consider a data collection of size n and denote them by $X_1, X_2, \ldots, X_n$. A graphical description, called a *histogram*, can be constructed by selecting a collection of class intervals of the form $[a_{k-1}, a_k) = \{x \ : \ a_{k-1} \leq x < a_k\}$ where $a_1 < a_2 < \ldots < a_K$ are numbers, and plotting bars over the intervals proportional to the number of data values n_k in the kth interval. In case the class intervals are not of equal length, we adjust the bar height h_k for the kth interval to take that into account. To be precise, we can construct the following table:

Table 1.1: Histogram Data

Class Interval	Length	Count	Proportion	Bar Height
$[a_0, a_1)$	$L_1 = a_1 - a_0$	n_1	$p_1 = n_1/n$	$h_1 = p_1/L_1$
$[a_1, a_2)$	$L_2 = a_2 - a_1$	n_2	$p_2 = n_2/n$	$h_2 = p_2/L_2$
$\ldots$	$\ldots$	$\ldots$	$\ldots$	$\ldots$
$[a_{K-1}, a_K)$	$L_K = a_K - a_{K-1}$	n_K	$p_K = n_K/n$	$h_K = p_K/L_K$

Note that $n_1 + n_2 + \cdots + n_K = n$ the total number, provided all the data are between a_0 and a_K.

To illustrate, consider the following $n = 111$ data values in table 1 corresponding to coded freezing dates of Lake Mendota in Madison Wisconsin:

Table 1.2: 111 Freezing Dates for Lake Mendota 1855-1965.
November 23 coded 0, ..., January 30 coded 68.

25	13	2	15	14	21	9	33	25	15	21	25	19	17	9	31
26	7	6	17	48	15	44	28	24	0	40	17	25	24	19	12
31	40	52	33	34	23	11	35	43	28	24	16	34	32	22	32
20	21	39	27	39	29	25	16	35	31	50	23	35	23	18	41
16	32	32	23	39	26	23	13	24	28	10	23	68	17	32	31
27	43	14	35	40	43	41	14	23	25	20	37	28	31	30	18
23	37	37	40	19	21	37	16	36	26	23	19	27	22	49	

If we select class intervals [0,10), [10,20), ..., [60,70) we get the following table:

Table 1.3: Data for Freezing Dates Histogram

Class Interval	Length	Count	Proportion	Bar Height
[0,10)	10	6	0.054	0.0054
[10,20)	10	25	0.225	0.0225
[20,30)	10	38	0.342	0.0342
[30,40)	10	27	0.243	0.0243
[40,50)	10	12	0.108	0.0108
[50,60)	10	2	0.018	0.0018
[60,70)	10	1	0.009	0.0009

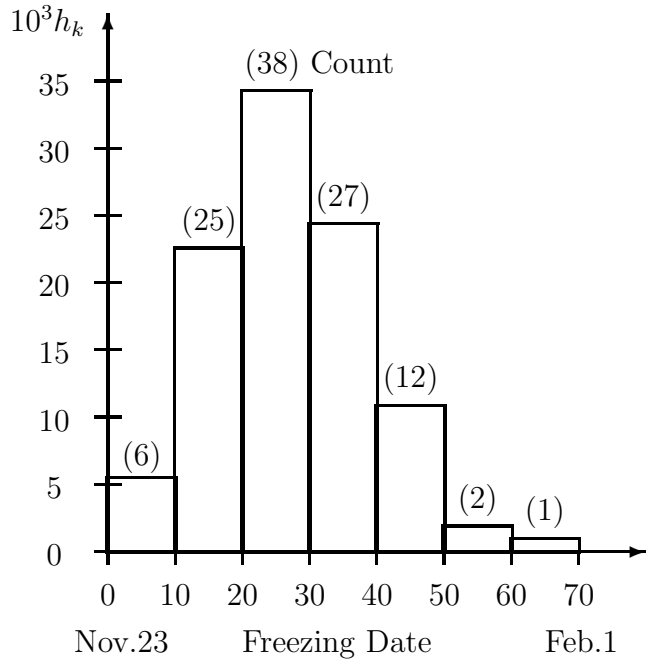

Figure 1.1: Histogram for Lake Mendota Freezing Data.

In order to give a specific choice for the number of class intervals K, and endpoint values a_k for the intervals, we follow the aesthetic histogram construction of Doane.[1]

Denote the data sorted into increasing order, by $X_{(1)}, X_{(2)}, \ldots, X_{(n)}$ where $X_{(1)} \leq X_{(2)} \leq \ldots \leq X_{(n)}$. These are the order statistics. Next define x to be *a very round number* if $x = A \times 10^B$ where $A = 1, 2,$ or 5 and B is any positive or negative integer. We say the *roundness* of a number L is the largest very round divisor of L. For example 700 is rounder than 695 since 700 is divisible by 100 and 695 is divisible by 5 with $100 > 5$. Next let $\lfloor x \rfloor$ be the largest integer not exceeding x. For example $\lfloor 3.2 \rfloor = 3$ and $\lfloor -4.8 \rfloor = -5$. Then to be precise

1. Choose $K = 1 + \lfloor \log_2(n) \rfloor$.

2. Select the roundest number L to satisfy $K \times L \geq X_{(n)} - X_{(1)} = R$ and $(K-1) \times L < R$.

[1] David P. Doane (1976) Aesthetic Frequency Classifications. *The American Statistician* **30, #4,** 181-183.

3. Choose the roundest number a_0 that satisfies $a_0 \leq X_{(1)}$ and $X_{(n)} < a_0 + K \times L$.

4. Let $a_k = a_0 + k \times L$ for $k = 0, 1, \ldots K$.

Consider the following $n = 111$ data values.

Table 1.4: 111 Thawing Dates for Lake Mendota 1855-1965. Nov. 23$\leftrightarrow$ 0.

143	164	123	111	124	138	141	137	150	133	146	148	129	144	140	130
152	151	142	143	139	145	106	140	123	161	118	141	144	148	147	143
144	128	127	144	131	135	112	136	134	138	124	146	145	139	127	121
146	129	136	121	122	135	123	117	143	130	138	138	137	139	133	123
126	113	128	148	143	147	147	116	130	124	117	121	133	132	123	125
128	141	119	132	145	139	123	130	137	117	118	138	132	127	139	140
137	149	122	132	133	132	132	142	141	134	140	131	140	142	114	

We illustrate the above four rules for constructing an aesthetic histogram with the data from table 1.3.

1. $K = 1 + \lfloor \log_2(111) \rfloor \doteq 1 + \lfloor 6.794 \rfloor = 7$.

2. The roundest L satisfying $7L \geq 164 - 106 = 58$ and $6L < 58$ is $L = 9$.

3. The roundest a_0 satisfying $a_0 \leq 106$ and $164 < a_0 + 63$ is $a_0 = 105$.

4. $a_k = 105 + 9k$ for $k = 0, 1, \ldots, 7$.

Table 1.5: Data for Thawing Dates Histogram

Class Interval	Length	Count	Proportion	Bar Height
[105,114)	9	4	0.0360	0.0040
[114,123)	9	13	0.1171	0.0130
[123,132)	9	25	0.2252	0.0250
[132,141)	9	35	0.3153	0.0350
[141,150)	9	29	0.2613	0.0290
[150,159)	9	3	0.0270	0.0030
[159,168)	9	2	0.0180	0.0020

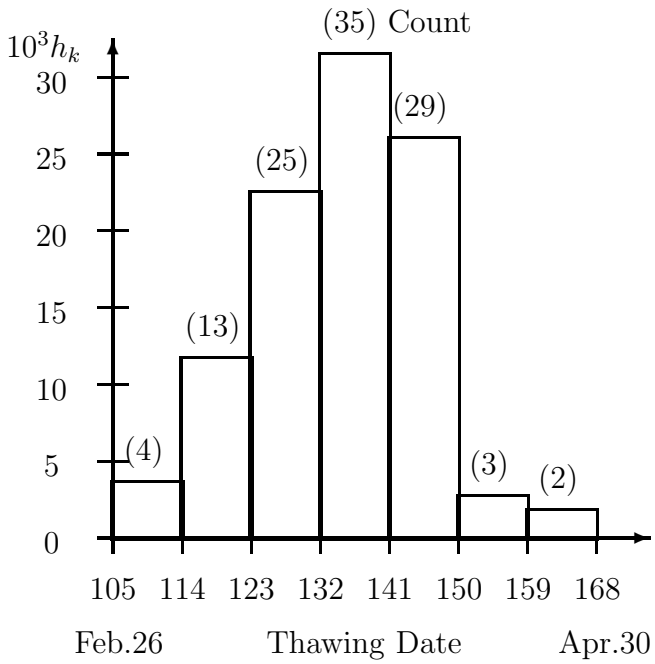

Figure 1.2: Histogram for Lake Mendota Thawing Data.

1.1.2 Stem-and-Leaf Diagrams

A stem-and-leaf diagram is a variation of the histogram in which the leading digits of the data values take the place of the class intervals and the low order digit is used to build the bar height. The stem-and-leaf diagram can reconstruct the order statistics. To illustrate the stem-and-leaf diagram for the freezing data, see table 1.6.

To subdivide the class intervals we can break the high order digits for the stem in two parts by listing low order digits 0,1,2,3,4 on one line and 5,6,7,8,9 on the next line. To illustrate for the thawing data, see table 1.7.

Subdivision into 5 parts uses 5 stems for {0,1}, {2,3},{4,5},{6,7},and {8,9} respectively.

Table 1.6: Stem-and-Leaf Diagram for Freezing Data

Stem	**Leaf**
0	026799
1	012334445556667777889999
2	00111122333333334444555556677788889
3	011111222223344555567777999
4	000011333489
5	02
6	8

Table 1.7: Stem-and-leaf Diagram for Thawing Data

Stem	**Leaf**
10	
10	6
11	1234
11	6777889
12	11122333333444
12	5677788899
13	000011222222333344
13	556677778888899999
14	000001111222333334444
14	5556667778889
15	012
15	
16	14
16	

1.1.3 Boxplots

To define a boxplot, we first define sample percentiles.

Definition. The 100p-th percentile is a value x such that the number of data values less than or equal x is at least $n \times p$ and the number of observations greater than or equal x is at least $n \times (1-p)$.

The 25th, 50th, and 75th percentiles are the lower (first) quartile, the second quartile (or median), and the upper (third) quartile. respectively. They are sometimes denoted Q_1, Q_2 (or $\tilde{X}$), and Q_3.

We define percentiles in terms of order statistics where the 100p-th percentile is, for integer r,

$$Z_p = \begin{cases} X_{(r)} & \text{if } r > np \text{ and } n-r+1 > n(1-p) \\ (X_{(r)} + X_{(r+1)})/2 & \text{if } r = np \end{cases}$$

The median, often denoted $\tilde{X}$, is defined by

$$\tilde{X} = \begin{cases} X_{(k+1)} & \text{for odd } n = 2k+1 \\ (X_{(k)} + X_{(k+1)})/2 & \text{for even } n = 2k \end{cases}$$

to be the middle or the average of the two middle data values after sorting. It is the 50th percentile using the interpolated definition.

We now can define a boxplot in terms of $X_{(1)}$, Q_1, $\tilde{X}$, Q_3, and $X_{(n)}$.

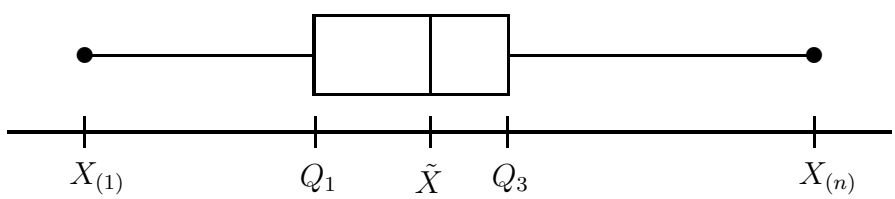

Figure 1.3: **Boxplot Using Quartiles.**

To illustrate for the Mendota thawing data, we have $X_{(1)} = 106$, $Q_1 = 126$, $\tilde{X} = 135$, $Q_3 = 142$ and $X_{(111)} = 164$ and the box plot is:

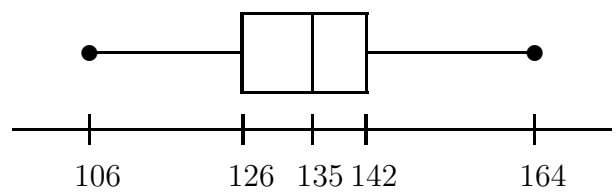

Figure 1.4: Boxplot for Mendota Thawing Data

1.1.4 Dot Diagrams

A dot diagram consists of dots placed on a line at locations corresponding to the value of each observation X_i for $i = 1, 2, \ldots, n$. For example, if the sorted data values are:
1.2, 2.3, 2.7, 2.7, 3.4, 3.6, 3.8, 3.8, 3.8, 3.8, 4.2, 4.2, 4.9, 5.4, 5.4, 6.1,7.2
then the corresponding dot diagram is:

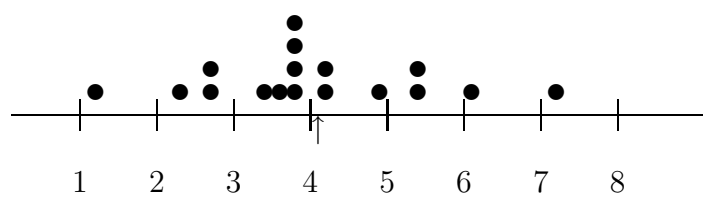

Figure 1.5: A Dot Diagram.

1.2 Measures of the Center

1.2.1 The Sample Median

Recall, the median $\tilde{X}$ is defined by

$$\tilde{X} = \begin{cases} X_{(k+1)} & \text{for odd } n = 2k+1 \\ (X_{(k)} + X_{(k+1)})/2 & \text{for even } n = 2k \end{cases}$$

to be the middle or the average of the two middle data values after sorting. It is the 50th percentile using the percentile definition. At least 50% of the

data values are less than or equal the median and at least 50% are greater than or equal the median. It is a *stable* measure of the center in that it is not much affected by an extreme value.

There are algorithms for calculating the median that are somewhat faster than a sorting algorithm ($\mathrm{O}(n)$ vs. $\mathrm{O}(n \log n)$. However, because of ready access to sorting algorithms such as *quicksort*, it seems simpler to calculate by sorting to obtain the order statistics and then select the middle one(s).

1.2.2 Some Robust Measures of the Center

The r-trimmed mean is designed to protect against a few wild observations and is defined by

$$T_r = \frac{X_{(r+1)} + X_{(r+2)} + \cdots + X_{(n-r-1)} + X_{(n-r)}}{(n-2r)}$$

It trims r observations from of each end of the sorted observations and averages the remaining values.

A modification is the r-Winsorized mean defined by

$$W_r = \frac{(r+1)X_{(r+1)} + X_{(r+2)} + \cdots + X_{(n-r-1)} + (r+1)X_{(n-r)}}{n}.$$

It replaces the r smallest observations by $X_{(r+1)}$ and the r largest values by $X_{(n-r)}$ and then averages.

Another robust estimator of the center is the Walsh sum median defined by first calculating all $n(n+1)/2$ Walsh sums

$$\frac{(X_i + X_j)}{2} \text{ for } 1 \le i \le j \le n$$

and then calculating the median

$$\tilde{M} = \text{median}\{(X_i + X_j)/2 \ : \ 1 \le i \le j \le n\}.$$

The Walsh sums are obtained from the following triangular array

$\frac{X_i+X_j}{2}$	X_1	X_2	X_3	$\cdots$	X_{n-1}	X_n
X_1	X_1	$\frac{X_1+X_2}{2}$	$\frac{X_1+X_3}{2}$	$\cdots$	$\frac{X_1+X_{n-1}}{2}$	$\frac{X_1+X_n}{2}$
X_2		X_2	$\frac{X_2+X_3}{2}$	$\cdots$	$\frac{X_2+X_{n-1}}{2}$	$\frac{X_2+X_n}{2}$
X_3			X_3	$\cdots$	$\frac{X_3+X_{n-1}}{2}$	$\frac{X_3+X_n}{2}$
$\vdots$				$\ddots$	$\vdots$	$\vdots$
X_{n-1}					X_{n-1}	$\frac{X_{n-1}+X_n}{2}$
X_n						X_n

and then sorted to find the median $\tilde{M}$ of these $n(n+1)/2$ values.

To illustrate the calculation of these three robust estimators consider the ten values
4.7, 1.2, 10.2, 6.2, 10.9, 1.4, 5.8, 1.1, 10.8, 5.1
Then the 2-trimmed mean is

$$T_2 = \frac{1.4 + 4.7 + 5.1 + 5.8 + 6.2 + 10.2}{6} \doteq 5.567 \ .$$

The 3-Winsorized mean is

$$W_3 = \frac{4 \times 4.7 + 5.1 + 5.8 + 4 \times 6.2}{10} \doteq 5.450 \ .$$

To calculate the Walsh sum median we first calculate the 55 Walsh sums:

$\frac{X_i+X_j}{2}$	4.7	1.2	10.2	6.2	10.9	1.4	5.8	1.1	10.8	5.1
4.7	4.70	2.95	7.45	5.45	7.80	3.05	5.25	2.90	7.75	4.90
1.2		1.20	5.70	3.70	6.05	1.30	3.50	1.15	6.00	3.15
10.2			10.20	8.20	10.55	5.80	8.00	5.65	10.50	7.65
6.2				6.20	8.55	3.80	6.00	3.65	8.50	5.65
10.9					10.90	6.15	8.35	6.00	10.85	8.00
1.4						1.40	3.60	1.25	6.10	3.25
5.8							5.80	3.45	8.30	5.45
1.1								1.10	5.95	3.10
10.8									10.8	7.95
5.1										5.10

The sorted Walsh sums are
1.1, 1.15, 1.2, 1.25, 1.3, 1.4, 2.9, 2.95, 3.05, 3.1, 3.15, 3.25, 3.45, 3.5, 3.6, 3.65, 3.7, 3.8, 4.7, 4.9, 5.1, 5.25, 5.45, 5.45, 5.65, 5.65, 5.7, **5.8**, 5.8, 5.95, 6, 6, 6, 6.05, 6.1, 6.15, 6.2, 7.45, 7.65, 7.75, 7.8, 7.95, 8, 8, 8.2, 8.3, 8.35, 8.5, 8.55, 10.2, 10.5, 10.55, 10.8, 10.85, 10.9
and the Walsh sum median is the middle value $\tilde{M} = 5.8$.

1.2.3 The Sample Mean or Average.

The most commonly used measure of the center is the sample mean or sample average defined by

$$\bar{X} = \frac{X_1 + X_2 + \cdots + X_n}{n} = \frac{\sum_{i=1}^{n} X_i}{n}.$$

If we put unit weights for each dot in the dot diagram, then the point of balance of the system of weights is at $\bar{X}$. For the dot diagram in figure 1.5, $\bar{X} = 4.0294$ as indicated by the arrow $\uparrow$. In contrast to the median and other robust estimators, the sample mean can be greatly affected by a single extreme value.

1.3 Measures of Dispersion or Spread

1.3.1 The Sample Range and Interquartile Range

The sample range is defined as the difference of the largest and smallest values. In terms of the order statistics,

$$R = X_{(n)} - X_{(1)}.$$

The interquartile range is defined by the difference of the third and first quartiles,

$$IQR = Q_3 - Q_1.$$

The larger the range values, the more dispersed are the data values.

1.3.2 Mean Absolute Deviation

The mean absolute deviation about the sample median is defined by

$$D = \frac{1}{n}\sum_{i=1}^{n} |X_i - \tilde{X}|.$$

Sometimes the sample mean $\bar{X}$ is used instead of the sample median $\tilde{X}$ but then the measure is larger.

1.3.3 The Sample Variance

The most commonly used measure of spread is the sample variance defined by

$$S^2 = \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{n-1}. \tag{1.1}$$

The square root $S = (S^2)^{1/2}$ is called the sample standard deviation.
Other equations which are formally equivalent but have different numerical accuracy are

$$S^2 = \frac{(\sum_{i=1}^{n} X_i^2) - n\bar{X}^2}{n-1} \tag{1.2}$$

$$S^2 = \frac{(\sum_{i=1}^{n} (X_i - C)^2) - n(\bar{X} - C)^2}{n-1} \tag{1.3}$$

for any constant C.
Finally, if we write $S^2 = S^2[n]$ and $\bar{X} = \bar{X}[n]$ to indicate the number of values used in the calculation, we have update equations

$$S^2[n] = \frac{(n-2)}{(n-1)} S^2[n-1] + \frac{1}{n}(\bar{X}[n-1] - X_n)^2 \tag{1.4}$$

$$\bar{X}[n] = \frac{X_n + \sum_{i=1}^{n-1} X_i}{n} = \frac{X_n + (n-1)\bar{X}[n-1]}{n}$$

with starting values $S^2[1] = 0$, $\bar{X}[1] = X_1$.

Equation (1.1) is an accurate method of calculating S^2 but requires two passes through the data. The first pass is used to calculate $\bar{X}$, and the second to calculate S^2 using $\bar{X}$.

Equation (1.2) is often used by programmers to calculate S^2 since it only requires one pass through the data. Unfortunately, it can be inaccurate due to subtraction of quantities with common leading digits ($\sum X_i^2$ and $n\bar{X}^2$).

A more accurate one pass method uses equation (1.4) although it is slightly more complicated to program.

Equation (1.3) is useful for data with many common leading digits. For example, using the values $(1000000001, 1000000002, 1000000003)$, we can take $C = 1000000000$ in (1.3) and calculate $S^2 = 1$, Many pocket calculators fail to get the correct answer for such values because of the use of equation (1.2).

To illustrate each calculation, consider the data $(X_1, X_2, \ldots, X_n) =$ $(2.0,\ 1.0,\ 4.0,\ 3.0,\ 5.0)$.

For equation (1.1) we first calculate $\bar{X} = (2+1+4+3+5)/5 = 3$ and then

$$S^2 = \frac{(2-3)^2 + (1-3)^2 + (4-3)^2 + (3-3)^2 + (5-3)^2}{(5-1)} = \frac{10}{4} = 2.5\ .$$

For equation (1.2) we have

$$S^2 = \frac{(2^2 + 1^2 + 4^2 + 3^2 + 5^2) - (5 \times 3^2)}{(5-1)} = \frac{55-45}{4} = 2.5 \ .$$

Using an arbitrary constant $C = 4$ equation (1.3) gives

$$\begin{aligned} S^2 &= \frac{[(2-4)^2 + (1-4)^2 + (4-4)^2 + (3-4)^2 + (5-4)^2] - [5 \times (3-4)^2]}{(5-1)} \\ &= \frac{15-5}{4} = 2.5 \ . \end{aligned}$$

For equation (1.4) starting with $n = 1$ and updating for $n = 2, 3, 4, 5$ we get

$$\begin{aligned} n &= 1 & \begin{cases} \bar{X}[1] = 2 \\ S^2[1] = 0 \end{cases} \\ n &= 2 & \begin{cases} \bar{X}[2] = (1+2)/2 = 1.5 \\ S^2[2] = 0 + (1/2)(2-1)^2 = 0.5 \end{cases} \\ n &= 3 & \begin{cases} \bar{X}[3] = (4 + 2 \times 1.5)/3 = 7/3 \\ S^2[3] = (1/2)0.5 + (1/3)(1.5-4)^2 = 7/3 \end{cases} \\ n &= 4 & \begin{cases} \bar{X}[4] = (3 + 3 \times 7/3)/4 = 2.5 \\ S^2[4] = (2/3)7/3 + (1/4)(7/3-3)^2 = 5/3 \end{cases} \\ n &= 5 & \begin{cases} \bar{X}[5] = (5 + 4 \times 2.5)/4 = 3 \\ S^2[5] = (3/4)5/3 + (1/5)(2.5-5)^2 = 2.5 \end{cases} \end{aligned} \tag{1.5}$$

1.4 Grouped Data

Sometimes there are many repetitions of data values and it is more convenient to represent the data in a table that gives the values and their counts as follows:

value	x_1	x_2	$\ldots$	x_K
counts	n_1	n_2	$\ldots$	n_K

where $x_1 < x_2 < \cdots < x_K$ and $n_1 + n_2 + \cdots + n_K = n$. The sample median is then

$$\tilde{X} = \begin{cases} x_r & \text{if } \sum_{i=1}^{r} n_i > n/2 \text{ and } \sum_{i=r}^{K} n_i > n/2 \\ (x_r + x_{r+1})/2 & \text{if } \sum_{i=1}^{r} n_i = n/2. \end{cases} \tag{1.6}$$

To calculate the r-trimmed mean and r-Winsorized mean for grouped data determine integers (s,t) for $r < n/2$ where $0 \le s < t \le K$, $\sum_{i=1}^{s} n_i \le r < \sum_{i=1}^{s+1} n_i$, and $\sum_{i=t+1}^{K} n_i \le r < \sum_{i=t}^{K} n_i$. Then

$$T_r = \frac{[(\sum_{i=1}^{s+1} n_i) - r]x_{s+1} + n_{s+2}x_{s+2} + \cdots + n_{t-1}x_{t-1} + [(\sum_{i=t}^{K} n_i) - r]x_t}{n - 2r} \tag{1.7}$$

$$W_r = \frac{(\sum_{i=1}^{s+1} n_i)x_{s+1} + n_{s+2}x_{s+2} + \cdots + n_{t-1}x_{t-1} + (\sum_{i=t}^{K} n_i)x_t}{n}. \tag{1.8}$$

For the Walsh sum median for grouped data, we construct the upper triangular table of Walsh sum values $\{w_{ij} = (x_i + x_j)/2 \ : \ \text{for } 1 \le i \le j \le K\}$

$(x_i + x_j)/2$	x_1	x_2	x_3	$\dots$	x_K
x_1	x_1	$(x_1 + x_2)/2$	$(x_1 + x_3)/2$	$\dots$	$(x_1 + x_K)/2$
x_2		x_2	$(x_2 + x_3)/2$	$\dots$	$(x_2 + x_K)/2$
x_3			x_3	$\dots$	$(x_3 + x_K)/2$
$\vdots$				$\ddots$	$\vdots$
x_K					x_K

These values are repeated with counts $n_{ij} = n_i(n_i + 1)/2$ for $i = j$ and $n_{ij} = n_i n_j$ for $i < j$:

counts	n_1	n_2	n_3	$\dots$	n_K
n_1	$n_1(n_1 + 1)/2$	$n_1 n_2$	$n_1 n_3$	$\dots$	$n_1 n_K$
n_2		$n_2(n_2 + 1)/2$	$n_2 n_3$	$\dots$	$n_2 n_K$
n_3			$n_3(n_3 + 1)/2$	$\dots$	$n_3 n_K$
$\vdots$				$\ddots$	$\vdots$
n_K					$n_K(n_K + 1)/2$

We then sort the $N = K(K+1)/2$ Walsh sum values w_{ij} along with their counts n_{ij} to get

sorted Walsh sums	$w_{(1)}$	$w_{(2)}$	$\dots$	$w_{(N)}$
corresponding counts	m_1	m_2	$\dots$	m_N

We then calculate the median $\tilde{M}$ using equation (1.6) applied to this table of values and counts. Note $w_{(1)} = x_1$, $m_1 = n_1(n_1+1)/2$, $w_{(2)} = (x_1 + x_2)/2$, $m_2 = n_1 n_2$, $\dots$, $w_{(N-1)} = (x_{K-1} + x_K)/2$, $m_{N-1} = n_{K-1} n_K$, $w_{(N)} = x_K$, $m_N = n_K(n_K + 1)/2$. The rest of the values must be determined by sorting.

We have the identity

$$\sum_{i=1}^{K} \frac{n_i(n_i+1)}{2} + \sum_{i=1}^{K-1}\sum_{j=i}^{K} n_i n_j = \sum_{i=1}^{K} \frac{n_i}{2} + \frac{1}{2}\sum_{i=1}^{K}\sum_{j=1}^{K} n_i n_j = \frac{n(n+1)}{2}$$

so that the count of the total number of Walsh sums agrees with that for the ungrouped case.

The sample mean for grouped data is the weighted average

$$\bar{X} = \frac{n_1 x_1 + n_2 x_2 + \cdots + n_K x_K}{n}. \tag{1.9}$$

For measures of spread the sample range is $R = x_K - x_1$ and the interquartile range is $IQR = Q_3 - Q_1$ where Q_1 is the 25th percentile and Q_3 is the 75th percentile. For grouped data, we define a 100p-th percentile by

$$Z_p = \begin{cases} x_r & \text{if } \sum_{i=1}^{r} n_i > np \text{ and } \sum_{i=r}^{K} n_i > n(1-p) \\ (x_r + x_{r+1})/2 & \text{if } \sum_{i=1}^{r} n_i = np\ . \end{cases}$$

Then $Q_1 = Z_{.25}$ and $Q_3 = Z_{.75}$

The mean absolute deviation about the median for grouped data is

$$D = \frac{\sum_{i=1}^{K} |n_i(x_i - \tilde{X})|}{n}$$

where $\tilde{X}$ is calculated from equation (1.6).

To calculate S^2 for grouped data we have formulae corresponding to equations (1.1), (1.2), (1.3), and (1.4) for ungrouped data.

$$S^2 = \frac{\sum_{i=1}^{K} n_i(x_i - \bar{X})^2}{n-1} \tag{1.10}$$

$$S^2 = \frac{(\sum_{i=1}^{K} n_i x_i^2) - n\bar{X}^2}{n-1} \tag{1.11}$$

$$S^2 = \frac{(\sum_{i=1}^{K} n_i(x_i - C)^2) - n(\bar{X} - C)^2}{n-1} \tag{1.12}$$

where $\bar{X}$ is calculated from equation (1.9).

For the update equation, write

$$S^2\{k\} = \frac{\sum_{i=1}^{k} n_i(x_i - \bar{X}\{k\})^2}{N\{k\} - 1}$$

where

$$\bar{X}\{k\} = \frac{\sum_{i=1}^{k} n_i x_i}{N\{k\}}, \quad N\{k\} = \sum_{i=1}^{k} n_i \ .$$

Then $S^2 = S^2\{K\}$, $\bar{X} = \bar{X}\{K\}$, $n = N\{K\}$, and

$$\bar{X}\{k\} = (n_k x_k + N\{k-1\}\bar{X}\{k-1\})/N\{k\}$$

$$S^2\{k\} = \left(\frac{N\{k-1\}-1}{N\{k\}-1}\right) S^2\{k-1\} + \frac{n_k N\{k-1\}}{N\{k\}(N\{k\}-1)}(\bar{X}\{k-1\} - x_k)^2 \tag{1.13}$$

for $k = 1, 2, \ldots, K$ with starting values $S^2\{1\} = 0,\ \bar{X}\{1\} = x_1,\ N\{1\} = n_1$.

To illustrate calculations for grouped data, consider the table

value	1.2	1.7	5.8	6.7	11.2	12.1
count	3	4	8	10	6	2

Then the median

$$\tilde{X} = 6.7$$

from equation (1.6) with $r = 4$ since $3 + 4 + 8 + 10 = 25 > 33 \times 0.5$ and $10 + 6 + 2 > 33 \times 0.5$.

The 5-trimmed mean is

$$T_5 = \frac{2 \times 1.7 + 8 \times 5.8 + 10 \times 6.7 + 3 \times 11.2}{23} \doteq 6.539$$

from equation (1.7).

The 7-Winsorized mean is

$$W_7 = \frac{15 \times 5.8 + 10 \times 6.7 + 8 \times 11.2}{33} \doteq 7.382$$

from equation (1.8).

To calculate the Walsh sum median we set up the arrays of values and counts

$\frac{x_i+x_j}{2}$	1.2	1.7	5.8	6.7	11.2	12.1
1.2	1.2	1.45	3.5	3.95	6.2	6.65
1.7		1.7	3.75	4.2	6.45	6.9
5.8			5.8	6.25	8.5	8.95
6.7				6.7	8.95	9.4
11.2					11.2	11.65
12.1						12.1

counts	3	4	8	10	6	2
3	6	12	24	30	18	6
4		10	32	40	24	8
8			36	80	48	16
10				55	60	20
6					21	12
2						3

We then sort the values, carrying along the corresponding counts to get the table

value	1.2	1.45	1.7	3.5	3.75	3.95	4.2	5.8	6.2	**6.25**	6.45
count	6	12	10	24	32	30	40	36	18	80	24

value	6.65	6.7	6.9	8.5	8.95	8.95	9.4	11.2	11.65	12.1
count	6	55	8	48	16	60	20	21	12	3

from which the median is $\tilde{M} = 6.25$ for these sorted Walsh sums.

The sample mean is

$$\bar{X} = \frac{3 \times 1.2 + 4 \times 1.7 + 8 \times 5.8 + 10 \times 6.7 + 6 \times 11.2 + 2 \times 12.1}{33} \doteq 6.521 \ .$$

For measures of spread we have

$$R = 12.1 - 1.2 = 10.9$$

$$IQR = 6.7 - 5.8 = 0.9$$

$$D = \sum_{i=1}^{K} n_i |x_i - \tilde{X}|/n \doteq 2.4697 \ .$$

To calculate S^2 using equations (1.10), (1.11), or (1.12) we obtain

$$S^2 \doteq 11.74985$$

Using the update equation (1.13) for grouped data we get

$$
\begin{aligned}
k &= 1 & \begin{cases} \bar{X}\{1\} = 1.2 \\ S^2\{1\} = 0 \end{cases} \\
k &= 2 & \begin{cases} \bar{X}\{2\} = (4 \times 1.7 + 3 \times 1.2)/7 \doteq 1.48571 \\ S^2\{2\} = \left(\frac{3-1}{7-1}\right) \times 0 + \frac{4\times 3}{7\times 6}(1.2 - 1.7)^2 \doteq 0.07143 \end{cases} \\
k &= 3 & \begin{cases} \bar{X}\{3\} = (8 \times 5.8 + 7 \times 1.48571)/15 \doteq 3.78667 \\ S^2\{3\} = \left(\frac{7-1}{15-1}\right) 0.07143 + \frac{8\times 7}{15\times 14}(1.48571 - 5.8)^2 \doteq 4.99411 \end{cases} \\
k &= 4 & \begin{cases} \bar{X}\{4\} = (10 \times 6.7 + 15 \times 3.78667)/25 \doteq 4.9520 \\ S^2\{4\} = \left(\frac{15-1}{25-1}\right) 4.99411 + \frac{10\times 15}{25\times 24}(3.78667 - 6.7)^2 \doteq 5.03510 \end{cases} \\
k &= 5 & \begin{cases} \bar{X}\{5\} = (6 \times 11.2 + 25 \times 4.9520)/31 \doteq 6.16129 \\ S^2\{5\} = \left(\frac{25-1}{31-1}\right) 5.03510 + \frac{6\times 25}{31\times 30}(4.9520 - 11.2)^2 \doteq 10.32445 \end{cases} \\
k &= 6 & \begin{cases} \bar{X}\{6\} = (2 \times 12.1 + 31 \times 6.16129)/33 \doteq 6.52121 \\ S^2\{6\} = \left(\frac{31-1}{33-1}\right) 10.32445 + \frac{2\times 31}{33\times 32}(6.16129 - 12.1)^2 \doteq 11.74985 \end{cases}
\end{aligned}
\tag{1.14}
$$

1.5 Properties

If the data values are transformed by a linear transformation

$$X_i \to aX_i + b$$

then these measures of the center transform in the same way

$$\tilde{X} \to a\tilde{X} + b, \quad T_r \to aT_r + b, \quad W_r \to aW_r + b, \quad \tilde{M} \to a\tilde{M} + b, \quad \bar{X} \to a\bar{X} + b.$$

The measures of dispersion transform as follows:

$$R \to |a|R, \quad IQR \to |a|IQR, \quad D \to |a|D$$

and

$$S \to |a|S, \quad S^2 \to a^2 S^2.$$

Proposition 1.1 *The sample median $\tilde{X}$ is the value C that minimizes $\sum_{i=1}^{n} |X_i - C|$.*

Proof.
Define $X_{(0)} = -\infty$ and $X_{(n+1)} = +\infty$.
Let $X_{(r)} < C \leq X_{(r+1)}$ for $r \in \{0, 1, \ldots n\}$.
Our proof considers two cases.
Case I. $\tilde{X} < C$.
For $n = 2k+1$ we have $\tilde{X} = X_{(k+1)} < C \leq X_{(r+1)}$ and $r > k$.
For $n = 2k$, $\tilde{X} = (X_{(k)} + X_{(k+1)})/2 < C \leq X_{(r+1)}$ and $r \geq k$.
Then

$$\sum_{i=1}^{n} |X_i - C| - \sum_{i=1}^{n} |X_i - \tilde{X}|$$

$$= \sum_{i=1}^{r} (C - X_{(i)}) + \sum_{i=r+1}^{n} (X_{(i)} - C) - \sum_{i=1}^{k} (\tilde{X} - X_{(i)}) - \sum_{i=k+1}^{n} (X_{(i)} - \tilde{X})$$

$$= \sum_{i=1}^{r} (C - \tilde{X} + \tilde{X} - C) + \sum_{i=r+1}^{n} (X_{(i)} - \tilde{X} + \tilde{X} - C) - \sum_{i=1}^{k} (\tilde{X} - X_{(i)}) - \sum_{i=k+1}^{n} (X_{(i)} - \tilde{X})$$

$$= (2r - n)(C - \tilde{X}) + 2 \sum_{i=k+1}^{r} (\tilde{X} - X_{(i)}) \ .$$

For $n = 2k+1$, since $(\tilde{X} - X_{(k+1)}) = 0$ we can sum from $k+2$. Using $X_{(k+1)} \leq X_{(k+2)} \leq \cdots \leq X_{(r)} < C$

$$(2r - n)(C - \tilde{X}) + 2 \sum_{i=k+2}^{r} (\tilde{X} - X_{(i)}) > (2k + 2 - n)(C - \tilde{X}) > 0$$

For $n = 2k$ similarly using $X_{(r)} < C$ replacing $X_{(i)}$ by C,

$$(2r - n)(C - \tilde{X}) + 2 \sum_{i=k+1}^{r} (\tilde{X} - X_{(i)}) > (2k - n)(C - \tilde{X}) = 0 \ .$$

Case II. $C \leq \tilde{X}$.
For $n = 2k+1$, $X_{(r)} < C \leq \tilde{X} = X_{(k+1)}$ gives $r < k+1$ or $r \leq k$.
For $n = 2k$, $X_{(r)} < C \leq \tilde{X} = (X_{(k)} + X_{(k+1)})/2$ also gives $r \leq k$.
Then as in case I and using $C \leq X_{(i)}$ for $i = r+1, r+2, \ldots, k$ we have

$$\sum_{i=1}^{n} |X_i - C| - \sum_{i=1}^{n} |X_i - \tilde{X}| = (2r - n)(C - \tilde{X}) + 2 \sum_{i=r+1}^{k} (X_{(i)} - \tilde{X}) \geq (n - 2k)(\tilde{X} - C) \geq 0$$

and $C = \tilde{X}$ minimizes in both cases. ■

Proposition 1.2 *The sample mean $\bar{X}$ is the value C that minimizes $\sum_{i=1}^{n}(X_i - C)^2$.*

Proof.

$$\sum_{i=1}^{n}(X_i - C)^2 = \sum_{i=1}^{n}(X_i - \bar{X} + \bar{X} - C)^2$$

$$= \sum_{i=1}^{n}(X_i - \bar{X})^2 + 2(\bar{X} - C)\sum_{i=1}^{n}(X_i - \bar{X}) + n(\bar{X} - C)^2$$

and using $\sum_{i=1}^{n}(X_i - \bar{X}) = 0$,

$$= \sum_{i=1}^{n}(X_i - \bar{X})^2 + n(\bar{X} - C)^2 \geq \sum_{i=1}^{n}(X_i - \bar{X})^2.$$

Thus $C = \bar{X}$ minimizes. ∎

Proposition 1.3 *If $C \geq 1$ then the proportion of observations outside the interval $(\tilde{X} - CD, \tilde{X} + CD)$ does not exceed $1/C$.*

Proof.
Let $\mathcal{A} = \{i \ : \ X_i \leq \tilde{X} - CD \text{ or } X_i \geq \tilde{X} + CD\}$. Then the proportion outside the interval is

$$\frac{\sum_{i \in \mathcal{A}} 1}{n} = \frac{1}{n} \sum_{\substack{i \, : \\ |X_i - \tilde{X}|/(CD) \geq 1}} 1 \leq \frac{1}{n}\sum_{i=1}^{n} |X_i - \tilde{X}|/(CD) = \frac{1}{C} \ . \ ∎$$

Proposition 1.4 (Chebyshev's Proposition for sample data).
If $C \geq 1$, then the proportion of observations outside the interval $(\bar{X} - CS, \bar{X} + CS)$ does not exceed $1/C^2$.

Proof.
Let $\mathcal{B} = \{i \ : \ X_i \leq \bar{X} - CS \text{ or } X_i \geq \bar{X} + CS\}$. Then the proportion outside the interval is

$$\frac{\sum_{i \in \mathcal{B}} 1}{n} = \frac{1}{n} \sum_{\substack{i \, : \\ (X_i - \bar{X})^2/(CS)^2 \geq 1}} 1 \leq \frac{1}{n}\sum_{i=1}^{n} (X_i - \bar{X})^2/(CS)^2 = \left(\frac{n-1}{nC^2}\right) \ . \ ∎$$

As an example, using $C = 10$, the proportion of data values outside of 10 standard deviations S from the sample mean does not exceed 1/100. This Chebyshev bound is usually quite crude and can be improved upon if the frequency distribution for the data is known.

An excellent statistical software package that can calculate many of the descriptive statistics as well as more complicated statistical procedures is R developed by Venables, Smith and the R Development Core Team. It can be downloaded from the web address **http:// www.r-project.org**. Manuals[2] are also available.

1.6 Problems

For problems (1)-(12) use the following data

12.5, 11.4, 10.5, 9.7, 15.2, 8.9, 7.6, 14.3,
13.1, 6.5, 17.0, 8.8, 7.7, 10.4, 11.0, 12.3

1. Construct the aesthetic histogram.

2. Construct a stem-and-leaf diagram.

3. Construct a box-plot.

4. Construct the dot diagram.

5. Calculate the sample median.

5. Calculate the 3-trimmed mean.

6. Calculate the 5-Winsorized mean.

7. Write a computer program to calculate the Walsh sum median.

8. Calculate the sample range R.

9. Calculate the inter quartile range IQR.

10. Calculate the mean absolute deviation about the median D.

[2]Venables, W.N., Smith, D.M. and the R Development Core Team (2004). *An Introduction to R*. A .pdf file available from **http:// www.r-project.org**

11. Calculate the sample variance S^2.

12. Write a computer program to calculate S^2 using the update formula (1.4).

13. Write a computer program to calculate the Walsh sum median for table 1.1.

For problems (14)-(17) use the following grouped data:

value	5.2	6.7	7.8	9.7	15.4
count	4	6	10	12	5

14. Calculate the sample median.

15. Calculate the Walsh sum median.

16. Calculate the sample mean.

17. Calculate S^2 using the update equation (1.13).

18. Prove formula (1.4).

19. Prove formula (1.13).

20. Prove $D \leq R/2$.

Chapter 2

Discrete Probability

2.1 The Sample Space

Consider a random experiment which has a variety of possible outcomes. Let us denote the set of possible outcomes, called the sample space, by

$$\mathcal{S} = \{e_1, e_2, e_3, \ldots\}.$$

If the outcome e_i belongs to the set $\mathcal{S}$ we write $e_i \in \mathcal{S}$. If the outcome does not belong to the set $\mathcal{S}$ we write $e \notin \mathcal{S}$.

Ws say the sample space is discrete if either there is a finite number of possible outcomes

$$\mathcal{S} = \{e_i \ : \ i = 1, 2, \ldots, n\}$$

or there is a countably infinite number of possible outcomes (the outcomes can be put into one to one correspondence with the set of positive integers)

$$\mathcal{S} = \{e_i \ : \ i = 1, 2, \ldots, \infty\}.$$

To illustrate, consider the random experiment of tossing a coin 3 times with each toss resulting in a heads (H) or a tail (T). Then the sample space is finite with

$$\mathcal{S} = \{HHH, HHT, HTH, THH, HTT, THT, TTH, TTT\}.$$

For another example, consider the random experiment of tossing a coin repeatedly until a heads (H) come up. Then the sample space is countably infinite with

$$\mathcal{S} = \{H, TH, TTH, TTTH, \ldots\}.$$

2.2 Events

Events are subsets of the sample space and we often use letters A, B, C, etc. to label them. For example in the finite sample space for the toss of a coin 3 times we might consider the event

$$A = \{HHT, HTH, THH\}$$

that 2 heads came up in 3 tosses. For the countable example, let the event B be an odd number of tosses occurred

$$B = \{H, TTH, TTTTH, TTTTTTH, \ldots\}.$$

2.2.1 Events Constructed From Other Events

Since we are dealing with subsets, set theory can be used to form other events.

The complement of an event A is defined by

$$A^c = \{e \ : \ e \in \mathcal{S} \text{ and } e \notin A\}.$$

It is the set of all outcomes in $\mathcal{S}$ that are not in A.

The intersection of two events A and B is defined by

$$A \cap B = \{e \ : \ e \in A \text{ and } e \in B\}.$$

It is the set of all outcomes common to both A and B. In case there are no outcomes common to both we say the intersection is empty and use the symbol $\phi = \{\ \}$ to represent the empty set (the set with no outcomes) and write $A \cap B = \phi$.

The union of two events is defined by putting them together

$$A \cup B = \{e \ : \ e \in A \text{ or } e \in B\}.$$

Here the word *or* is used in a non exclusive sense. The outcome in the union could belong to A, it could belong to B, or it could belong to both.

Intersections of multiple events such as a finite sequence of events or a countable sequence:

$$\{A_i \ : \ i = 1, 2, \ldots, N\} \text{ or } \{A_i \ : \ i = 1, 2, \ldots, \infty\}$$

are denoted by

$$\bigcap_{i=1}^{N} A_i = \{e \ : \ e \in A_i \text{ for all } i = 1, 2, \ldots, N\}$$

for finite intersections, and

$$\bigcap_{i=1}^{\infty} A_i = \{e \ : \ e \in A_i \text{ for all } i = 1, 2, \ldots, \infty\}$$

for countably infinite intersections. Similarly, we denote

$$\bigcup_{i=1}^{N} A_i = \{e \ : \ e \in A_i \text{ for some } i,\ i = 1, 2, \ldots, N\}$$

for finite unions, and

$$\bigcup_{i=1}^{\infty} A_i = \{e \ : \ e \in A_i \text{ for some } i,\ i = 1, 2, \ldots, \infty\}$$

for countably infinite unions.

To illustrate these definitions, consider the sample space for the roll of two dice . The first die is red and the second die is green and each die has 1,2,3,4,5, 6 on the faces. Then if we use the notation (i, j) where $i, j \in \{1, 2, 3, 4, 5, 6\}$ for an outcome with the first coordinate representing the up face for the red die and the second coordinate the up face for the green die, the sample space is

$$\begin{array}{lllllll}
\mathcal{S} = \{ & (1,1), & (1,2), & (1,3), & (1,4), & (1,5), & (1,6), \\
 & (2,1), & (2,2), & (2,3), & (2,4), & (2,5), & (2,6), \\
 & (3,1), & (3,2), & (3,3), & (3,4), & (3,5), & (3,6), \\
 & (4,1), & (4,2), & (4,3), & (4,4), & (4,5), & (4,6), \\
 & (5,1), & (5,2), & (5,3), & (5,4), & (5,5), & (5,6), \\
 & (6,1), & (6,2), & (6,3), & (6,4), & (6,5), & (6,6) \ \}
\end{array}$$

Let the event A be *the 1st (red) die is 3 or less*

$$\begin{array}{lllllll}
A = \{ & (1,1), & (1,2), & (1,3), & (1,4), & (1,5), & (1,6), \\
 & (2,1), & (2,2), & (2,3), & (2,4), & (2,5), & (2,6), \\
 & (3,1), & (3,2), & (3,3), & (3,4), & (3,5), & (3,6)\}
\end{array}$$

Let B be the event *the sum is divisible by 3*

$$B = \{\ (1,2),\ (2,1),\ (1,5),\ (2,4),\ (3,3),\ (4,2),\ (5,1),$$
$$(3,6),\ (4,5),\ (5,4),\ (6,3),\ (6,6)\}\ .$$

Then the complement of A is

$$\begin{array}{rllllll} A^c = \{ & (4,1), & (4,2), & (4,3), & (4,4), & (4,5), & (4,6), \\ & (5,1), & (5,2), & (5,3), & (5,4), & (5,5), & (5,6), \\ & (6,1), & (6,2), & (6,3), & (6,4), & (6,5), & (6,6)\ \}\ . \end{array}$$

The intersection of A and B is

$$A \cap B = \{\ (1,2),\ (2,1),\ (1,5),\ (2,4),\ (3,3),\ (3,6)\ \}\ .$$

The union of A, B is

$$\begin{array}{rllllll} A \cup B = \{ & (1,1), & (1,2), & (1,3), & (1,4), & (1,5), & (1,6), \\ & (2,1), & (2,2), & (2,3), & (2,4), & (2,5), & (2,6), \\ & (3,1), & (3,2), & (3,3), & (3,4), & (3,5), & (3,6), \\ & (4,2), & (4,5), & (5,1), & (5,4), & (6,3), & (6,6)\ \}\ . \end{array}$$

2.2.2 Event Relations

We say the event A is a subset of B and write $A \subset B$ if and only if $e \in A$ implies $e \in B$. That is B has all the outcomes that A has (and possibly others). In symbols

$$A \subset B \Longleftrightarrow \{e \in A \Longrightarrow e \in B\}\ .$$

We say that two sets $A,\ B$ are equal if both $A \subset B$ and $B \subset A$.
DeMorgan's rules.

$$(a)\quad (A \cup B)^c = (A^c) \cap (B^c), \quad (b)\quad (A \cap B)^c = (A^c) \cup (B^c)\ .$$

Proof. We show outcomes in the left set belong to the right set and conversely.
(a)

$$e \in (A \cup B)^c \Longleftrightarrow e \notin (A \cup B) \Longleftrightarrow \{e \notin A\} \text{ and } \{e \notin B\}$$
$$\Longleftrightarrow \{e \in A^c\} \text{ and } \{e \in B^c\} \Longleftrightarrow e \in (A^c) \cap (B^c).\ \blacksquare$$

(b)

$$e \in (A \cap B)^c \Longleftrightarrow e \notin (A \cap B) \Longleftrightarrow \{e \notin A\} \text{ or } \{e \notin B\}$$

$$\Longleftrightarrow \{e \in A^c\} \text{ or } \{e \in B^c\} \Longleftrightarrow e \in (A^c) \cup (B^c). \blacksquare$$

Distributive laws.

$(a) \quad A \cap (B \cup C) = (A \cap B) \cup (A \cap C), \quad (b) \quad A \cup (B \cap C) = (A \cup B) \cap (A \cup C)$.

Proof.
(a)

$$e \in A \cap (B \cup C) \Longleftrightarrow \{e \in A\} \text{ and } \{e \in (B \cup C)\}$$

$$\Longleftrightarrow \{e \in A\} \text{ and } \{\{e \in B\} \text{ or } \{e \in C\}\}$$

$$\Longleftrightarrow \{\{e \in A\} \text{ and } \{e \in B\}\} \text{ or } \{\{e \in A\} \text{ and } \{e \in C\}\}$$

$$\Longleftrightarrow \{e \in A \cap B\} \text{ or } \{e \in A \cap C\} \Longleftrightarrow e \in (A \cap B) \cup (A \cap C). \blacksquare$$

(b)

$$e \in A \cup (B \cap C) \Longleftrightarrow \{e \in A\} \text{ or } \{e \in (B \cap C)\}$$

$$\Longleftrightarrow \{e \in A\} \text{ or } \{\{e \in B\} \text{ and } \{e \in C\}\}$$

$$\Longleftrightarrow \{\{e \in A\} \text{ or } \{e \in B\}\} \text{ and } \{\{e \in A\} \text{ or } \{e \in C\}\}$$

$$\Longleftrightarrow \{e \in A \cup B\} \text{ and } \{e \in A \cup C\} \Longleftrightarrow e \in (A \cup B) \cap (A \cup C). \blacksquare$$

DeMorgan's rules and the distributive laws also hold for finite or infinite collections of events:

$$(\bigcup_{i=1}^{N} A_i)^c = \bigcap_{i=1}^{N} A_i^c \ , \quad (\bigcup_{i=1}^{\infty} A_i)^c = \bigcap_{i=1}^{\infty} A_i^c$$

$$(\bigcap_{i=1}^{N} A_i)^c = \bigcup_{i=1}^{N} A_i^c \ , \quad (\bigcap_{i=1}^{\infty} A_i)^c = \bigcup_{i=1}^{\infty} A_i^c \ .$$

$$B \cap (\bigcup_{i=1}^{N} A_i) = \bigcup_{i=1}^{N} (B \cap A_i) \ , \quad B \cup (\bigcap_{i=1}^{N} A_i) = \bigcap_{i=1}^{N} (B \cup A_i) \ .$$

$$B \cap (\bigcup_{i=1}^{\infty} A_i) = \bigcup_{i=1}^{\infty} (B \cap A_i) \ , \quad B \cup (\bigcap_{i=1}^{\infty} A_i) = \bigcap_{i=1}^{\infty} (B \cup A_i) \ .$$

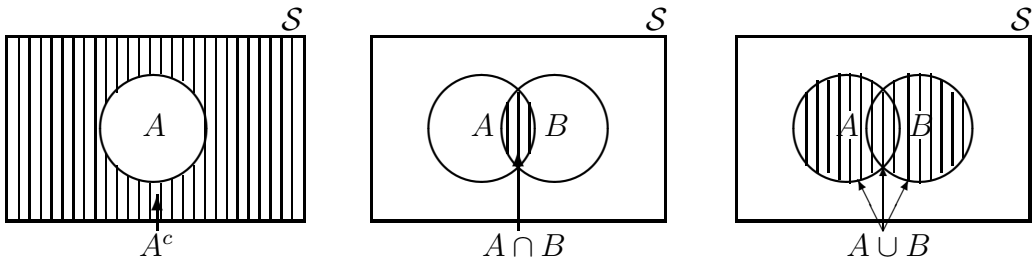

Figure 2.1: Three Venn diagrams illustrating A^c, $A \cap B$, and $A \cup B$.

2.2.3 Venn Diagrams

Venn diagrams are a graphical method to visualize set relations. We use a bounding rectangle to represent the sample space S and closed curves such as circles to represent events $A,\ B,\ C, \cdots$. We can shade regions to represent sets of interest. For example, the three Venn diagrams above illustrate A^c, $A \cap B$, and $A \cup B$ shaded with vertical lines.

2.2.4 Sigma Fields of Events

Before defining probabilities for events we discuss the collection of events on which we define the probability. Such a collection is a class of sets $\mathcal{A}$ with the following properties:

(i). $\mathcal{S} \in \mathcal{A}$.

(ii). If $A \in \mathcal{A}$ then $A^c \in \mathcal{A}$.

(iii). if $A_i \in \mathcal{A}$ for $i = 1, 2, \ldots, \infty$ then $\bigcup_{i=1}^{\infty} A_i \in \mathcal{A}$.

Using (i) and (ii) we have $\phi = \mathcal{S}^c \in \mathcal{A}$.
If $A_i \in \mathcal{A}$ for $i = 1, 2, \ldots, \infty$ then $\bigcap_{i=1}^{\infty} A_i \in \mathcal{A}$ using DeMorgan's rule and (ii),(iii)

$$\bigcap_{i=1}^{\infty} A_i = (\bigcup_{i=1}^{\infty} A_i^c)^c \in \mathcal{A}\ .$$

Using the infinite sequence $\{A_i \ : \ i = 1, 2, \ldots, \infty\}$ where $A_i = \phi$ for $i = N+1, N+2, \ldots, \infty$ we have using (iii)

$$\bigcup_{i=1}^{N} A_i = \bigcup_{i=1}^{\infty} A_i \in \mathcal{A} \ .$$

Then using this finite union, DeMorgan's rule, and (ii),(iii) we have

$$\bigcap_{i=1}^{N} A_i = (\bigcup_{i=1}^{N} A_i^c)^c \in \mathcal{A}$$

and finite unions and intersections belong to $\mathcal{A}$ as well as countably infinite unions and intersections. Thus our class of events $\mathcal{A}$ is a rich collection and we cannot get a set outside of it by taking complements unions, or intersections. This class is called a **sigma field**.

2.3 Probability

Intuitively, the probability of an event A, denoted $P(A)$, is a number such that $0 \leq P(A) \leq 1$ with 1 indicating that the event is certain to occur, and 0 that it will not. There are several philosophical interpretations of probability. For the **Bayesian** school of probability, the probability represents their personal belief of the frequency of occurence. Different Bayesians may assign different probabilities to the same event. For the **frequentist** school, probability represents the limiting average frequency of occurrence of the event in repeated trials of identical random experiments as the number of trials goes to infinity. Other philosophies, use symmetry or other considerations to assign probability.

For any interpretation, we require that a probability is a measure for events in a sigma field and satisfies the following axioms due to Kolmogorov, the late famous Russian probabilist:
(i). $0 \leq P(A) \leq 1$.
(ii). If $\{A_i \ : \ i = 1, 2, \ldots, \infty, \ A_i \cap A_j = \phi \text{ for } i \neq j\}$ then

$$P(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i) \ .$$

This is called sigma additivity for disjoint events.
(iii). $P(\mathcal{S}) = 1$.
From these axioms, all properties of a probability are derived.

Lemma 2.1 $P(\phi) = 0$

Proof. If $P(\phi) > 0$, then

$$P(\phi) = P(\bigcup_{i=1}^{\infty} \phi) = \sum_{i=1}^{\infty} P(\phi) = \infty$$

by (ii), and gives the contradiction to (i) that $P(\phi) = \infty$. ■

Lemma 2.2 *For a finite collection of events that are disjoint*

$$\{A_i \ : \ i = 1, 2, \ldots, N, \ A_i \cap A_j = \phi \textit{ for } i \neq j\}$$

$$P(\bigcup_{i=1}^{N} A_i) = \sum_{i=1}^{N} P(A_i)$$

Proof. Consider the countable sequence of events

$$\{A_i \ : \ i = 1, 2, \ldots, \infty, \ A_i \cap A_j = \phi \text{ for } i \neq j\}$$

where $A_i = \phi$ for $i = N+1, N+2, \ldots, \infty$ we have

$$P(\bigcup_{i=1}^{N} A_i) = P(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} P(A_i) = \sum_{i=1}^{N} P(A_i)$$

and finite additivity holds for disjoint events. ■

Lemma 2.3 $P(A^c) = 1 - P(A)$.

Proof. Using $\mathcal{S} = A \cup A^c$, where $A \cap A^c = \phi$, and finite additivity

$$1 = P(\mathcal{S}) = P(A \cup A^c) = P(A) + P(A^c) \ .$$

Subtracting $P(A)$ from both sides gives the result. ■

Lemma 2.4 *If $A \subset B$, then $A = A \cap B$ and $P(A) \leq P(B)$.*

Proof.

$$e \in A \Longrightarrow e \in A \text{ and } e \in B \Longrightarrow e \in A \cap B \ .$$

Converseley

$$e \in A \cap B \Longrightarrow e \in A \text{ and } e \in B \Longrightarrow e \in A$$

so that $A = A \cap B$.
Next using the distributive law for events

$$P(B) = P(B \cap \mathcal{S}) = P(B \cap (A \cup A^c)) = P((B \cap A) \cup (B \cap A^c))$$

and using $A = A \cap B$ and finite additivity for disjoint A and $B \cap A^c$

$$= P(A \cup (B \cap A^c)) = P(A) + P(B \cap A^c) \geq P(A) \ . \blacksquare$$

Lemma 2.5 *If $A, B \in \mathcal{A}$ are any two sets, not necessarily disjoint, then*

$$P(A \cup B) = P(A) + P(B) - P(A \cap B) \ . \tag{2.1}$$

Proof. Using the distributive law for events, let

$$A \cup B = (A \cap \mathcal{S}) \cup (B \cap \mathcal{S}) = (A \cap (B \cup B^c)) \cup (B \cap (A \cup A^c))$$

$$= (A \cap B) \cup (A \cap B^c) \cup (B \cap A) \cup (B \cap A^c) = (A \cap B^c) \cup (A \cap B) \cup (B \cap A^c)$$

Then by finite additivity for disjoint events

$$P(A \cup B) = P(A \cap B^c) + P(A \cap B) + P(B \cap A^c) \ .$$

Adding and subtracting $P(A \cap B)$ and using finite additivity gives

$$= (P(A \cap B^c) + P(A \cap B)) + (P(B \cap A^c) + P(A \cap B)) - P(A \cap B)$$

$$= P(A) + P(B) - P(A \cap B) \ . \blacksquare$$

Lemma 2.6 *For a finite sequence of not necessarily disjoint events $\{A_i \ : \ i = 1, 2, \ldots, N, \ \}$ we have*

$$P(\bigcup_{i=1}^{N} A_i) = \sum_{i=1}^{N} (-1)^{i-1} S_i^{(N)} \tag{2.2}$$

where

$$\begin{aligned}
S_1^{(N)} &= \sum_{i=1}^{N} P(A_i) \\
S_2^{(N)} &= \sum_{1\le i<j\le N}\sum P(A_i \cap A_j) \\
S_3^{(N)} &= \sum_{1\le i<j<k\le N}\sum\sum P(A_i \cap A_j \cap A_k) \\
\dots &= \dots \\
S_N^{(N)} &= P(\bigcap_{i=1}^{N} A_i)
\end{aligned}$$

Proof by induction. For $N = 1$ equation (2.2) reduces to the identity $P(A_1) = P(A_1)$.
For $N = 2$ we get $P(A_1 \cup A_2) = P(A_1) + P(A_2) - P(A_1 \cap A_2)$ which holds by equation (2.1).
Now assume the induction hypothesis that (2.2) holds for $N = m$ events, to show that it also holds for $N = m + 1$.

$$P(\bigcup_{i=1}^{m+1} A_i) = P((\bigcup_{i=1}^{m} A_i) \cup A_{m+1}) = P(\bigcup_{i=1}^{m} A_i) + P(A_{m+1}) - P(A_{m+1} \cap (\bigcup_{i=1}^{m} A_i))$$

using (2.1). Applying the distributive law to the last term and (2.2) for m events to the first and last terms we get

$$P(\bigcup_{i=1}^{m+1} A_i) = \sum_{i=1}^{m}(-1)^{i-1}S_i^{(m)} + P(A_{m+1}) - \sum_{i=1}^{m}(-1)^{i-1}S_i^{(m)}(m+1)$$

where

$$S_i^{(m)}(m+1) = \sum\sum\dots\sum_{1\le j_1<j_2<\dots<j_i\le m} P(\bigcap_{k=1}^{i}(A_{m+1} \cap A_{j_k}))\ .$$

Using

$$S_1^{(m+1)} = S_1^{(m)} + P(A_{m+1})\ , \quad (-1)^m S_{m+1}^{(m+1)} = -(-1)^{m-1}S_m^{(m)}(m+1)\ ,$$

and

$$(-1)^{i-1}S_i^{(m+1)} = (-1)^{i-1}S_i^{(m)} - (-1)^{i-2}S_{i-1}^{(m)}(m+1) \text{ for } i = 2, 3, \dots, m\ ,$$

we get (2.2) holds for $N = m + 1$ events which completes the induction:

$$P(\bigcup_{i=1}^{m+1} A_i) = \sum_{i=1}^{m+1} (-1)^{i-1} S_i^{(m+1)} \ . \ \blacksquare$$

2.3.1 Defining Probability for Discrete Sample Spaces

For the discrete case $\mathcal{S} = \{e_1,\ e_2,\ e_3, \ldots\}$, where there are a finite or countably infinite number of outcomes, we use the sigma field of all possible subsets of $\mathcal{S}$ including $\phi, \mathcal{S}$. We assign numbers $p_i \geq 0$ to each outcome e_i where $\sum_{\{i\,:\,e_i \in \mathcal{S}\}} p_i = 1$. We then define

$$P(A) = \sum_{\substack{i\,:\\ e_i \in A}} p_i$$

This definition satisfies the probability axioms.
Axiom (i) holds since $p_i \geq 0$ and $P(\mathcal{S}) = 1$, we have

$$0 \leq \sum_{\substack{i\,:\\ e_i \in A}} p_i = P(A) \leq \sum_{\substack{i\,:\\ e_i \in \mathcal{S}}} p_i = P(\mathcal{S}) = 1 \ .$$

Axiom (ii) holds since we can break up the sums for disjoint events $\{A_i \ : \ i = 1, 2, \ldots, \infty$ where $A_i \cap A_j = \phi$ for $i \neq j\}$. Note, for finite sample spaces, all but a finite number of the sets are the empty set ϕ. For these we use the convention that a sum over no outcomes is zero.

$$P(\bigcup_{i=1}^{\infty} A_i) = \sum_{\substack{j\,:\\ e_j \in \bigcup_{i=1}^{\infty} A_i}} p_j = \sum_{i=1}^{\infty} \sum_{\substack{j_i\,:\\ e_{j_i} \in A_i}} p_{j_i} = \sum_{i=1}^{\infty} P(A_i) \ .$$

Finally, axiom (iii) holds since $P(\mathcal{S}) = \sum_{\{i\,:\,e_i \in \mathcal{S}\}} p_i = 1$.

As an example, consider the sample space $\mathcal{S} = \{H,\ TH,\ TTH,\ TTTH, \ldots\}$ of tossing a coin until it comes up heads. Suppose we assign corresponding probabilities $\{1/2,\ 1/4,\ 1/8,\ \ldots\}$ where $p_i = (1/2)^i$. Then if the event B is *an odd number of tosses*, $B = \{H,\ TTH,\ TTTTH, \ldots\}$, we have

$$P(B) = \sum_{\substack{i\,:\\ e_i \in B}} \left(\frac{1}{2}\right)^{2i-1} = \frac{1}{2} + \frac{1}{8} + \frac{1}{32} + \ldots$$

$$= \frac{1}{2}\sum_{k=0}^{\infty}\left(\frac{1}{4}\right)^k = \frac{1}{2}\frac{1}{(1-\frac{1}{4})} = \frac{2}{3}$$

using the geometric series identity $\sum_{k=0}^{\infty} x^k = 1/(1-x)$, $0 < x < 1$, for $x = 1/4$.

2.3.2 Equal Probabilities in Finite Sample Spaces

An important special case is that of a finite sample space $\mathcal{S} = \{e_1,\ e_2,\ e_3, \ldots, e_N\}$ with associated probabilities $p_i = 1/N$ for all outcomes e_i, $i = 1, 2, \ldots, N$. Then if we denote the number of outcomes in the set A by $||A||$ we have

$$P(A) = \sum_{\substack{i\,:\\ e_i \in A}} \frac{1}{N} = \frac{1}{N}\sum_{\substack{i\,:\\ e_i \in A}} 1 = \frac{||A||}{||\mathcal{S}||}\ .$$

For such probabilities, it is necessary to count the number of outcomes $||A||$ and $||\mathcal{S}|| = N$. We give some standard counting rules.

Rule 2.1 Product rule.
If one operation can be done in n_1 ways and the second operation can be done in n_2 ways independently of the first operation then the pair of operations can be done in $n_1 \times n_2$ ways.
If we have K operations, each of which can be done independently in n_k ways for $k = 1, 2, \ldots, K$ then the combined operation can be done in $n_1 \times n_2 \times \cdots \times n_K$ ways.

For example, a touring bicycle has a derailleur gear with 3 front chainwheels and a rear cluster with 9 sprockets. A gear selection of a front chainwheel and a rear sprocket can be done in $3 \times 9 = 27$ ways.
A combination lock has 40 numbers on the dial $0, 1, 2, \ldots, 39$. A setting consists of 3 numbers. This can be done in $40 \times 40 \times 40 = 64,000$ ways.

Rule 2.2 Permutation rule.
The number of different possible orderings of r items taken from a total of n items is $n(n-1)(n-2)\cdots(n-r+1)$. We denote this by $(n)_r$. Other notations are ${}_nP_r$ and P_r^n. For the special case of $r = n$ we use the notation $n!$ and read it n-factorial.

Proof. Applying the product rule, the first item can be chosen in n ways, then independently of this choice, there are $(n-1)$ ways to choose the 2nd item, $(n-2)$ ways for the third, ..., $(n-r+1)$ ways for the rth choice. ■

For example, if the items are $\{1,\ 2,\ 3,\ 4,\ 5\}$ the different arrangements of 3 items are

(1,2,3), (1,3,2), (2,1,3), (2,3,1), (3,1,2), (3,2,1)
(1,2,4), (1,4,2), (2,1,4), (2,4,1), (4,1,2), (4,2,1)
(1,2,5), (1,5,2), (2,1,5), (2,5,1), (5,1,2), (5,2,1)
(1,3,4), (1,4,3), (3,1,4), (3,4,1), (4,1,3), (4,3,1)
(1,3,5), (1,5,3), (3,1,5), (3,5,1), (5,1,3), (5,3,1)
(1,4,5), (1,5,4), (4,1,5), (4,5,1), (5,1,4), (5,4,1)
(2,3,4), (2,4,3), (3,2,4), (3,4,2), (4,2,3), (4,3,2)
(2,3,5), (2,5,3), (3,2,5), (3,5,2), (5,2,3), (5,3,2)
(2,4,5), (2,5,4), (4,2,5), (4,5,2), (5,2,4), (5,4,2)
(3,4,5), (3,5,4), (4,3,5), (4,5,3), (5,3,4), (5,4,3)

a total of $5 \times 4 \times 3 = 60$ different orderings.

The value of $n!$ can get very large. Some examples are

n	0	1	2	3	4	5	6	7	8	9
$n!$	1	1	2	6	24	120	720	5040	40320	362880

To approximate the value for large n, a refined Stirlings's approximation can be used

$$n! \doteq (2\pi)^{1/2} n^{n+1/2} e^{-n+1/(12n)} \ .$$

Next, consider the number of different subsets of size r from n different items, with the order of the items within the subset not distinguished.

Rule 2.3 Combination rule.
The number of different subsets of size r chosen from a set of n different items is

$$\binom{n}{r} = \frac{(n)_r}{r!}$$

which is called the number of combinations of n things taken r at a time. Other notations are ${}_nC_r$ and C_r^n. This is also the number of distinguishable arrangements of r elements of one type and $n-r$ elements of another type

Proof. Denote this number by x. Then if we consider the number of permutations of r items out of n total, we have the identity

$$(n)_r = x \times r!$$

since each unordered set of r items can be ordered in $(r)_r = r!$ ways to get the complete ordered collection. We divide by $r!$ to solve for x. For the proof of the second proposition, there is a one to one correspondence between selecting a subset and a sequence of two types of elements (identify the selected components in the subset with the position of the first type of element in the sequence).■

For the previous permutation example with $n = 5$ and $r = 3$ we can choose just one element from each line (e.g. in increasing order) to get the subsets

$$\{1,2,3\},\ \{1,2,4\},\ \{1,2,5\},\ \{1,3,4\}, \{1,3,5\},\ \{1,4,5\},$$

$$\{2,3,4\},\ \{2,3,5\},\ \{2,4,5\},\ \{3,4,5\}\ .$$

a total of $\begin{pmatrix} 5 \\ 3 \end{pmatrix} = (5)_3/3! = 60/6 = 10$ subsets. For two types of elements (say 0 or 1) we have corresponding sequences

$$11100,\ 11010,\ 11001,\ 10110,\ 10101,\ 10011,$$

$$01110,\ 01101,\ 01011,\ 00111\ .$$

We can also write

$$\begin{pmatrix} n \\ r \end{pmatrix} = \frac{(n)_r}{r!} = \frac{n!}{r!(n-r)!}$$

because of the cancellation of the last $n - r$ terms in $n!$ by $(n - r)!$ to get $(n)_r = n!/(n - r)!$. This shows the symmetry

$$\begin{pmatrix} n \\ r \end{pmatrix} = \begin{pmatrix} n \\ n-r \end{pmatrix}$$

and simplifies calculation by restricting to cases of $\min\{r, (n - r)\} \leq n/2$.

The combination is also called a binomial coefficient from the identity for powers of a binomial expression

$$(x + y)^n = \sum_{r=0}^{n} \begin{pmatrix} n \\ r \end{pmatrix} x^r y^{n-r}\ .$$

We use the conventions $\begin{pmatrix} n \\ 0 \end{pmatrix} = 1$, and $\begin{pmatrix} n \\ a \end{pmatrix} = 0$ for $a < 0$.

There are many identities for binomial coefficients. One is

$$\begin{pmatrix} n \\ r \end{pmatrix} + \begin{pmatrix} n \\ r-1 \end{pmatrix} = \begin{pmatrix} n+1 \\ r \end{pmatrix} .$$

This identity yields Pascal's triangle for building up a table of values:

$\begin{pmatrix} n \\ r \end{pmatrix}$	r									
	0	1	2	3	4	5	6	7	8	9
n										
1	1									
2	1	2	1							
3	1	3	3	1						
4	1	4	6	4	1					
5	1	5	10	10	5	1				
6	1	6	15	20	15	6	1			
7	1	7	21	35	35	21	7	1		
8	1	8	28	56	70	56	28	8	1	
9	1	9	36	84	126	126	84	36	9	1

$\cdots$

Rule 2.4 Multinomial Rule.
If we have K different types of elements of which there are n_k of type k for $k = 1, 2, \ldots, K$ and $\sum_{k=1}^{K} n_k = N$, then there are

$$\frac{N!}{\prod_{k=1}^{K}(n_k!)} = \begin{pmatrix} N \\ n_1 \end{pmatrix} \begin{pmatrix} N - n_1 \\ n_2 \end{pmatrix} \cdots \begin{pmatrix} N - n_1 - n_2 - \cdots - n_{K-2} \\ n_{K-1} \end{pmatrix}$$

distinguishable arrangements. It is called the multinomial coefficient and occurs in powers of a multinomial $(x_1 + x_1 + \cdots + x_K)^N$ as coefficient of $x_1^{n_1} x_2^{n_2} \cdots x_K^{n_K}$ in the expansion.

Proof. We use the product rule and the combination rule for sequences after dividing the group into the first type and the non first types. Then divide the non first types into the 2nd type and the non first or second types, and continue this process to get the right side of the above expression. Cancellation gives the factorial expression. ■

With these counting rules we consider a variety of examples.

In the first deal of 5 cards in a poker hand, what is the probability of a full house (3 of one kind and 2 of of another, e.g. 3 kings and 2 aces)? Using the product rule, permutation rule, and combination rule we have

$$P(\text{full house}) = \frac{(13)_2 \times \binom{4}{3} \times \binom{4}{2}}{\binom{52}{5}} = \frac{1872}{2598960} \doteq 7.202881 \times 10^{-4}$$

Order is important chosing 2 from the 13 card types $\{A, 2, 3, 4, 5, 6, 7, 8, 9, 10, J, Q, K\}$, (3 kings and 2 aces are different than 2 kings and 3 aces) but not within the 4 suits $\{\clubsuit, \spadesuit, \heartsuit, \diamondsuit\}$.

Assuming 365 days in a year, what is the probability of the event A_n that no two people out of a total of n have the same birthday?

$$P(A_n) = \frac{(365)_n}{365^n} \ .$$

The following is a table of values calculated starting with $P(A_1) = 1$ and updating with $P(A_n) = P(A_{n-1}) \times (366 - n)/365$:

n :	1	2	3	4	5	6	7	8	9	10	11	12
$P(A_n)$:	1	.9973	.9918	.9836	.9729	.9595	.9438	.9257	.9054	.8831	.8589	.8330

n :	13	14	15	16	17	18	19	20	21	22	23	24
$P(A_n)$:	.8056	.7769	.7471	.7164	.6850	.6531	.6209	.5886	.5563	.5243	.4927	.4617

This result that only 23 people make the probability less than 1/2 is surprising to many.

A postman has n identical junk mail flyers to place in mail boxes and does it at random instead of by address. What is the probability that at least one person gets the correct address?
Let A_i be the event of a match for the ith mailbox. To calculate $P(\bigcup_{i=1}^n A_i)$.

$$P(\bigcup_{i=1}^n A_i) = \sum_{i=1}^n (-1)^{i-1} S_i^{(n)}$$

using (2.2). We have

$$P(A_i) = 1/n, \quad P(A_i \cap A_j) = \frac{1}{(n)_2}, \quad P(\bigcap_{i=j_1}^{j_k} A_i) = \frac{1}{(n)_k}$$

and

$$S_k = \frac{\binom{n}{k}}{(n)_k} = \frac{1}{k!}$$

since there are $\binom{n}{k}$ terms in the sum each with value $1/(n)_k$. Then

$$P(\bigcup_{i=1}^{n} A_i) = 1 - \frac{1}{2!} + \frac{1}{3!} - \ldots + (-1)^{n-1}\frac{1}{n!} = \sum_{k=1}^{n}(-1)^{k-1}\frac{1}{k!} \ .$$

For large n, this is approximated by $1 - e^{-1} \doteq 0.6321$ using the Taylor series expansion for $e^{-1} = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!}$ where $e \doteq 2.71828$.

There are N different pairs of shoes in a dark closet. If $2K$ shoes are selected at random, $2K < N$, what is the probability $P(A_m)$ of getting m complete pairs where $0 \leq m \leq K$?

If we line up the N pairs of shoes there are $\binom{N}{m}$ ways to select m pairs. Among the remaining $N - m$ pairs we select $2K - 2m$ single shoes, either a left shoe or a right shoe. This can be done in $\binom{N-m}{2K-2m} \times 2^{2K-2m}$ ways. Thus

$$P(A_m) = \frac{\binom{N}{m} \times \binom{N-m}{2K-2m} \times 2^{2K-2m}}{\binom{2N}{2K}} \ .$$

What is the probability of getting 2 pairs in the first deal of a 5 card poker hand?

$$P(2 \text{ pairs}) = \frac{\binom{13}{2}\binom{4}{2}^2 11 \binom{4}{1}}{\binom{52}{5}} = \frac{123552}{2598960} \doteq 0.047539 \ .$$

Note, the order of selecting the pairs is unimportant.

How many different arrangements are possible for the letters in the word MISSISSIPPI? With type M we have $n_1 = 1$, type I has $n_2 = 4$, type S has $n_3 = 4$, and type P has $n_4 = 2$. So there are

$$\frac{11!}{1!4!4!2!} = 11 \times 210 \times 15 = 34650 \ .$$

Gamblers often quote probabilities in terms of *odds*. We say the odds in favor of an event A are m to n if $P(A) = m/(m+n)$.

2.4 Conditional Probability

Sometimes, the probability of an event is changed by knowing that another event has occurred. To reflect this change we define the conditional probability of an event A given that we know the event B has occurred and denote this $P(A|B)$. To illustrate the situation using Venn diagrams as in figure 2.2, we have the original sample space for the event A and then a reduced sample space restricted to the event B as follows: We rescale the probabilities for A in the new sample space of B so that the probabilities are 0 outside of B and proportional to the original probabilities within B. We take

$$P(A|B) = \sum_{\substack{i\,:\\ e_i \in A \cap B}} (C \times p_i) = C \times P(A \cap B)$$

where the constant of proportionality $C > 0$. We determine C by the requirement that $P(B|B) = 1$ which gives

$$P(B|B) = \sum_{\substack{i\,:\\ e_i \in B \cap B}} (C \times p_i) = C \times P(B) = 1 \ .$$

So $C = 1/P(B)$ and our definition becomes

$$P(A|B) = \frac{P(A \cap B)}{P(B)} \ .$$

Note, we require $P(B) > 0$ for this definition.

For an example, in the first deal of a 5 card poker hand, let A be the event of a flush (all 5 cards are from the same suit). Let B be the event that all 5 cards are red $\{\heartsuit, \diamondsuit\}$. Then

$$P(A) = \frac{4 \times \begin{pmatrix} 13 \\ 5 \end{pmatrix}}{\begin{pmatrix} 52 \\ 5 \end{pmatrix}} = \frac{5148}{2598960} \doteq 0.0019808$$

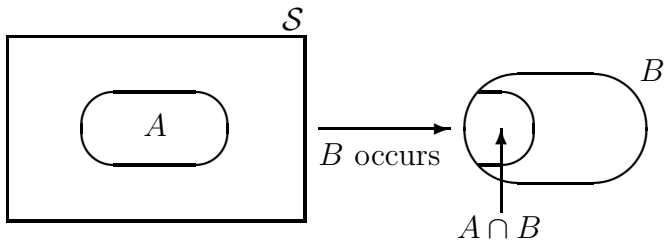

Figure 2.2: Changing Sample Space for Conditional Probability.

and

$$P(A|B) = \frac{2 \times \binom{13}{5} / \binom{52}{5}}{\binom{26}{5} / \binom{52}{5}} = \frac{2 \times \binom{13}{5}}{\binom{26}{5}} = \frac{2574}{65780} \doteq 0.039130 \ .$$

The probability of A knowing B has occurred increases, in this case, since mixtures with black cards have been ruled out.

An important theorem for conditional probabilities is

Bayes Theorem.

Let the sample space be partitioned into disjoint subsets

$$\mathcal{S} = \bigcup_{k=1}^{K} B_k \text{ where } B_j \cap B_k = \phi \text{ for } j \neq k \ .$$

Then for any event A we have

$$P(B_k|A) = \frac{P(A|B_k)P(B_k)}{\sum_{j=1}^{K} P(A|B_j)P(B_j)} \ .$$

Proof.

$$P(B_k|A) = \frac{P(A \cap B_k)}{P(A)} = \frac{P(A|B_k)P(B_k)}{P(A \cap S)}$$

$$= \frac{P(A|B_k)P(B_k)}{P(A \cap (\bigcup_{j=1}^{K} B_j))} = \frac{P(A|B_k)P(B_k)}{\sum_{j=1}^{K} P(A \cap B_j)} = \frac{P(A|B_k)P(B_k)}{\sum_{j=1}^{K} P(A|B_j)P(B_j)} \ . \blacksquare$$

As an example, suppose the incidence of disease in a population is $0.0001 = 1/10,000$. A screening test for the disease has a false positive error probability of 0.05 and a false negative error probability of 0.04. An individual

tests positive for the disease. What is the probability that the person has the disease?
Let B_1 be the event that the person has the disease, B_2 that the person does not, and A the event of being positive for the disease on the screening test. Then

$$P(B_1|A) = \frac{P(A|B_1)P(B_1)}{\sum_{j=1}^{2} P(A|B_j)P(B_j)} = \frac{(1-0.04)\times 0.0001}{0.96\times 0.001 + 0.05\times 0.9999} \doteq 0.001917\ .$$

Note that the probability is still not large although it is a factor of 19.17 larger than the population incidence. So don't panic but follow it up.

2.4.1 Independent Events

For the case when $P(A|B) = P(A)$, that is knowing B has occurred does not affect the probability of A, we say that the events A and B are *independent*. This condition can also be written $P(A \cap B) = P(A)P(B)$ for A and B independent.

We say the events $\{A_1,\ A_2, \ldots, A_n\}$ are *pairwise independent* if $P(A_i \cap A_j) = P(A_i)P(A_j)$ for all i, j with $i \neq j$.

We say the events $\{A_1,\ A_2, \ldots, A_n\}$ are *mutually independent* if we have

$$P(\bigcap_{i=j_1}^{j_k} A_i) = \prod_{i=j_1}^{j_k} P(A_i) \text{ for } j_1 < j_2 < \ldots < j_k \text{ and all } k = 2, 3, \ldots, n\ .$$

It is possible to have pairwise independence but not mutual independence. As an example, consider the sample space for the roll of two dice with probability 1/36 for each outcome. Let the event A_1 be first die odd, A_2 be the second die odd, and A_3 be the sum is odd. Then

$$P(A_1 \cap A_2) = \frac{9}{36} = \left(\frac{18}{36}\right)\left(\frac{18}{36}\right) = P(A_1)P(A_2)$$

$$P(A_1 \cap A_3) = \frac{9}{36} = \left(\frac{18}{36}\right)\left(\frac{18}{36}\right) = P(A_1)P(A_3)$$

$$P(A_2 \cap A_3) = \frac{9}{36} = \left(\frac{18}{36}\right)\left(\frac{18}{36}\right) = P(A_2)P(A_3)$$

And we have pairwise independence. Since the sum of two odd numbers is even,

$$P(A_1 \cap A_2 \cap A_3) = 0 \neq \left(\frac{18}{36}\right)\left(\frac{18}{36}\right)\left(\frac{18}{36}\right) = P(A_1)P(A_2)P(A_3)$$

and we do not have mutual independence.

The most common structure for independence is that of a sample space that is a product space. That is we have two sample collections $\{\mathcal{S}_1, \mathcal{A}_1, P_1\}$ and $\{\mathcal{S}_2, \mathcal{A}_2, P_2\}$ of the sample space, sigma field of events, and probability and we form a compound $\{\mathcal{S}, \mathcal{A}, P\}$ where the Cartesian product

$$\mathcal{S} = \{(e_i, e_j) \ : \ e_i \in \mathcal{S}_1, \ e_j \in \mathcal{S}_2\} \stackrel{def}{=} \mathcal{S}_1 \otimes \mathcal{S}_2$$

is the set of all pairs made up of outcomes from each individual sample space,

$$\mathcal{A} = \sigma\{A_1 \otimes A_2 \ : \ A_1 \in \mathcal{A}_1, \ A_2 \in \mathcal{A}_2\}$$

is the smallest sigma field that contains product sets (e.g. rectangles) from each individual sigma field, and P is determined by

$$P(A_1 \otimes A_2) = P_1(A_1)P_2(A_2) \text{ for } A_1 \in \mathcal{A}_1 \ , \quad A_2 \in \mathcal{A}_2 \ .$$

Events in $\mathcal{A}$ that are of the form $A_1 \otimes \mathcal{S}_2$ where $A_1 \in \mathcal{A}_1$ will be independent of events of the form $\mathcal{S}_1 \otimes A_2$ where $A_2 \in \mathcal{A}_2$.

In the example with the roll of two dice let $\mathcal{S}_1 = \{1, \ 2, \ 3, \ 4, \ 5, \ 6\}$, $\mathcal{A}_1$ be the class of all $2^6 = 16$ subsets of $\mathcal{S}_1$ including $\phi, \mathcal{S}_1$, $P_1(\{i\}) = 1/6$ for $i = 1, 2, \ldots, 6$ corresponding to the first die and similarly define $\{\mathcal{S}_2, \ \mathcal{A}_2, \ P_2\}$ for the second die. Then for the product space of the roll of the two dice

$$\mathcal{S} = \{(i, j) \ : \ i \in \mathcal{S}_1, \ \ j \in \mathcal{S}_2\} \text{ and } P(\{(i, j)\}) = \left(\frac{1}{6}\right)\left(\frac{1}{6}\right) = \frac{1}{36} \ .$$

In this example, the structure says that the roll of one die does not affect the other.

2.5 Problems

1. A white rook is placed at random on a chessboard. A black rook is then placed at random at one of the remaining squares. What is the probability that the black rook can capture the white rook?

2. Jack and Jill are seated randomly at a pair of chairs at an 11 chair round table. What is the probability that they are seated next to each other?

3. In a 7 game playoff series between team A and team B, the first to win 4 games wins the series. For each team, the probability of a win at home is 0.6 and away it is 0.4. Team A plays the first 2 games at home, then the next 3 away and then 2 at home if necessary. What is the probability that team A wins the series?

4. An old Ford trimotor airplane has engines on the left wing (L), on the right wing (R) and in the nose (N). The palne will crash if at least one wing engine and the nose engine fail. If the probabilities of failure are $P(L) = 0.05 = P(R)$ for the wing engines and $P(N) = 0.04$ for the nose engine, give the probability of a crash.

5. In 7 card stud poker, if only 5 cards can be used to make a poker hand, give the probability of a full house.

6. A soft drink case has 24 different slots. There are 3 coke bottles, 7 pepsi bottles, and 8 Dr. Pepper bottles. How many distinguishable ways can they be placed in the case?

7. How many distinguishable ways can 7 identical balls be placed in 11 different cells?

8. How many dominos are there in a set?

9. In a family with two children, what is the probability that both children are girls given that at least one is a girl?

10. A die is rolled and then a coin is tossed the number of times that the die came up. What is the probability that the die came up 5 given that 2 heads were observed to occur?

11. Prove DeMorgan's rules for an infinite collection of events.

12. Prove that the intersection of two sigma fields on the same sample space is a sigma field.

13. Prove by induction that the probability of exactly k of the events $\{A_1,\ A_2,\ \ldots, A_n\}$ occuring is given by

$$P_{[k]} = \sum_{i=k}^{n} (-1)^{k-i} \begin{pmatrix} i \\ k \end{pmatrix} S_i^{(n)} \ .$$

14. A fair coin is tossed until the same result occurs twice. Give the probability of an odd number of tosses.

15. A thick coin can come up heads (H), tails (T), or edge (E) with probabilities p_H, p_T, or p_E where $p_H + p_T + p_E = 1$.
(a) If the coin is tossed 4 times, describe the sample space of possible outcomes and assign probabilities assuming independence.
(b) Give the probability of getting 2 heads and 1 tail.

Chapter 3

Random Variables

We now consider numerical features of outcomes in the sample space and introduce the concept of a *random variable*.

Definition 3.1 *A random variable X is a function from the sample space $\mathcal{S}$ to the real line $R = \{x\ ;\ -\infty < x < \infty\} = (-\infty,\ \infty)$. For each outcome*

$$e \in \mathcal{S} \text{ we have } X(e) = x \text{ where } x \text{ is a number } -\infty < x < \infty\ .$$

Because we want to define probabilities we have

Definition 3.2 *A measurable random variable X is a random variable such that for each interval $B = (a, b] = \{x\ :\ a < x \leq b\}$ we have*

$$A = X^{-1}(B) = \{e\ :\ X(e) \in B\} \in \mathcal{A}\ .$$

That is, the set of all outcomes $A \subset \mathcal{S}$ that are mapped by X into the interval B on the real line belong to the sigma field $\mathcal{A}$ and so have a probability defined.

Definition 3.3 *The probability distribution $P_X(B)$ for a measurable random variable X is defined by*

$$P_X(B) = P(A) \text{ where } A = X^{-1}(B) \text{ for } B = (a, b]\ .$$

For general sets B in the Borel sigma field $\mathcal{B}$, which is the smallest sigma field that contains intervals, we define $P_X(B) = P(A)$ where $A = X^{-1}(B) \in \mathcal{A}$ by limits using the axioms.

Definition 3.4 *The sigma field $\mathcal{A}(X)$ of a measurable random variable is defined by*

$$\mathcal{A}(X) = \{A \ : \ A = X^{-1}(B) \text{ where } B \in \mathcal{B}\} \ .$$

Inverse inages of intervals in R determine the subsets A of $\mathcal{A}(X) \subset \mathcal{A}$.

To illustrate, consider the sample space of tossing a coin 3 times:

$$\mathcal{S} = \{HHH, HHT, HTH, THH, HTT, THT, TTH, TTT\}.$$

with associated probability 1/8 for each outcome. Define X to be the number of heads observed. Then

$$X(HHH) = 3, \ X(HHT) = X(HTH) = X(THH) = 2,$$

$$X(HTT) = X(THT) = X(TTH) = 1, \ X(TTT) = 0$$

and

$$P(X = x) = \begin{pmatrix} 3 \\ x \end{pmatrix} \frac{1}{8} \text{ for } x = 0, 1, 2, 3.$$

For the example of rolling two dice, let X be the sum of the two up faces. Then $X(i, j) = i + j$ for $i, j = 1, 2, \ldots, 6$ and

x	2	3	4	5	6	7	8	9	10	11	12
$P(X = x)$	$\frac{1}{36}$	$\frac{2}{36}$	$\frac{3}{36}$	$\frac{4}{36}$	$\frac{5}{36}$	$\frac{6}{36}$	$\frac{5}{36}$	$\frac{4}{36}$	$\frac{3}{36}$	$\frac{2}{36}$	$\frac{1}{36}$

For the example of tossing a coin until heads come up with $P(H) = 1/2 = P(T)$, if X is the nimber of tosses, $P(X = x) = (1/2)^x$ for $x = 1, 2, \ldots, \infty$.

3.1 Discrete Random Variables

A discrete random variable takes on only a finite or countably infinite number of values. The probability of such values is called the discrete *probability density function* (p.d.f.) and is often denoted by $f_X(x) = P(X = x)$ where x ranges over the possible values.

We consider some important such random variables.

3.1.1 Binomial Random Variables

Consider the sample space of tossing a bent coin n times with outcome probabilites determined by $P(H) = p$ and $P(T) = 1 - p = q$ where $0 < p < 1$. Then

$$P(\underbrace{HHH\cdots H}_{x}\underbrace{TTT\cdots T}_{n-x}) = p^x q^{n-x}$$

and similarly for all outcomes with x H's and $n - x$ T's. Then if X is the number of heads observed we have

$$P(X = x) = \begin{pmatrix} n \\ x \end{pmatrix} p^x q^{n-x} \text{ for } x = 0, 1, 2, \ldots, n$$

since there are $\begin{pmatrix} n \\ x \end{pmatrix}$ such outcomes with probability $p^x q^{n-x}$. This distribution is called the binomial distribution. The probabilities add to 1 since

$$\sum_{x=0}^{n} \begin{pmatrix} n \\ x \end{pmatrix} p^x q^{n-x} = (p + q)^n = 1^n = 1 \ .$$

3.1.2 Negative Binomial Random Variables

For tossing a coin repeatedly until r heads come up where the outcome probabilities are determined by $P(H) = p$ and $P(T) = 1-p = q$ let Y be the number of tails observed along the way. Then each outcome is of the form

$$\underbrace{HTTHH\ldots T|H}_{\text{r } H\text{'s and } y\ T\text{'s}}$$

with the last outcome the final rth head. This sequence has probability $p^r q^y$ and there are $\begin{pmatrix} y + r - 1 \\ y \end{pmatrix}$ such outcomes applying the binomial counting rule for sequences of two types of elements to the first $r - 1$ H's and y T's . Thus

$$P(Y = y) = \begin{pmatrix} y + r - 1 \\ y \end{pmatrix} p^r q^y \text{ for } y = 0, 1, 2, \ldots, \infty \ .$$

It gets its name from the coefficients in the negative binomial expansion $(p + q)^{-r}$. The probabilities add to 1 since

$$\sum_{y=0}^{\infty} \begin{pmatrix} y + r - 1 \\ y \end{pmatrix} p^r q^y = (p + q)^{-r} = 1^{-r} = 1 \ .$$

The special case where $r = 1$ is called the *geometric distribution*.

3.1.3 Poisson Distribution

For the binomial distribution with n large and p small but $\lambda = np$ moderate, the following Poisson distribution is a good approximation.

$$P(X = x) = \frac{\lambda^x}{x!} e^{-\lambda} \text{ for } x = 0, 1, 2, \ldots, \infty \ .$$

In fact we can show that the binomial with $n \to \infty$, $p = p_n \to 0$, $np_n \to \lambda$ converges to the Poisson. Writing the binomial probability as follows and using $(n)_x p_n^x \to \lambda^x$ and $(1 - p_n)^{n-x} \to e^{-\lambda}$ gives

$$\binom{n}{x} p_n^x (1 - p_n)^{n-x} = \frac{(n)_x p_n^x}{x!} (1 - p_n)^{n-x} \to \frac{\lambda^x}{x!} e^{-\lambda} \ .$$

3.1.4 Hypergeometric Distribution

The hypergeometric distribution often arises in a sampling situation where the sampling is done *without replacement*.

Consider an urn with a total of N items of which D are defective and $N-D$ are nondefective. We take out n items and observe the random variable X the number of defectives among the n selected without replacement. As in the binomial distribution there are $\binom{n}{x}$ sequences with x defectives and $n - x$ nondefectives among the n selected. However, since we do not replace items after selecting them, each such sequence has probability $(D)_x (N - D)_{n-x} / (N)_n$. Thus

$$f_X(x) = \binom{n}{x} \frac{(D)_x (N - D)_{n-x}}{(N)_n} = \frac{n! D! (N - n)! (N - D)!}{x! (n - x)! (D - x)! (N - n - D + x)! N!}$$

$$= \frac{\binom{n}{x}\binom{N-n}{D-x}}{\binom{N}{D}} = \frac{\binom{D}{x}\binom{N-D}{n-x}}{\binom{N}{n}} \text{ for } x = L, L+1, \ldots, U$$

where the limits are $L = \max\{0, n + D - N\}$ and $U = \min\{n, D\}$.
If we represent the urn items in figure 3.1, the last two expressions above can

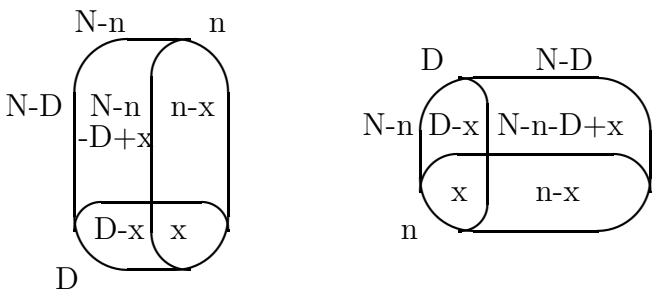

Figure 3.1: Division of Sample Space for Hypergeometric Distribution.

be viewed as partitioning into defectives and non defectives and then sampling and nonsampling for the left one and then partitioning into sampling and nonsampling then defective and nondefective selection for the right.

3.1.5 Negative Hypergeometric Distribution

For the urn with D defectives and $N - D$ nondefectives we sample without replacement until we get a total of r defectives. Let Y be the total nondefectives observed. Then the p.d.f. is

$$f_Y(y) = \binom{r+y-1}{y} \frac{(D)_r (N-D)_y}{(N)_{r+y}} = \frac{\binom{D}{r-1}\binom{N-D}{y}}{\binom{N}{r+y-1}} \frac{(D-(r-1))}{(N-y-(r-1))}$$

for $y = 0, 1, \ldots, N - D$, and $r \leq D$.

3.1.6 Cumulative Distribution Functions

The cumulative distribution function (c.d.f.) of a random variable X is defined by

$$F_X(x) = P(X \leq x) \ .$$

For discrete random variables, it is the sum of p.d.f. values up to and including x.

$$F_X(x) = \sum_{y \leq x} p_X(y) \ .$$

For integer valued random variables such as the binomial, negative binomial, Poisson, hypergeometric, and negative hypergeometric we have

$$P(a \leq X \leq b) = F_X(b) - F_X(a-1) \ .$$

To evaluate the c.d.f. for the Binomial, we can use its relationship to the area under the curve defined for $a, b > 0$ by

$$I_x(a,b) = \frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)} \int_0^x u^{a-1}(1-u)^{b-1} du$$

which is called the incomplete beta function. The gamma function $\Gamma(a) = \int_0^\infty u^{a-1}e^{-u}du$ and satisfies $\Gamma(n+1) = n!$, for integer n, $\Gamma(1/2) = (\pi)^{1/2}$, and $\Gamma(a+1) = a\Gamma(a)$ for $a > 0$. For the binomial, with parameters n and p

$$F_X(x; n, p) = \sum_{k=0}^{x} \binom{n}{k} p^k (1-p)^{n-k} = I_q(n-x, x+1)$$

The negative binomial c.d.f. can also be calculated using the incomplete beta function from

$$F_Y(y; r, p) = \sum_{k=0}^{y} \binom{k+r-1}{k} p^r q^k = I_p(r, y+1) \ .$$

For the Poisson c.d.f. we can use the incomplete gamma function given by

$$G(x, a) = \int_0^x \frac{u^{a-1}e^{-u}}{\Gamma(a)} du$$

and

$$\sum_{k=0}^{x} \frac{e^{-\lambda}\lambda^k}{k!} = 1 - G(\lambda, x+1) \ .$$

If we denote the hypergeometric c.d.f. by

$$F_X(x; N, D, n) = \sum_{k=L}^{x} \binom{n}{x} \frac{(D)_x (N-D)_{n-x}}{(N)_n}$$

where $L = \max\{0, n+D-N\}$ and integer $x \leq U = \min\{n, D\}$, then the negative hypergeometric c.d.f. can be expressed in terms of the hypergeometric by

$$F_Y(y; N, D, r) = \sum_{k=0}^{y} \binom{r+k-1}{k} \frac{(D)_r (N-D)_k}{(N)_{r+k}} = 1 - F_X(r-1; N, D, r+y) \ .$$

The C++ subroutines **cdf.h** in **Appendix A** gives programs that calculate these c.d.f.'s.

The incomplete beta function calculation uses an algorithm of Soper[1]. For $x \le a/(a+b)$ and $a, b \ge 1$ it uses the identity

$$I_x(a,b) = x^a(1-x)^{b-1}\frac{\Gamma(a+b)}{\Gamma(a+1)\Gamma(b)} + I_x(a+1,b-1)$$

a total of $S = \lfloor b + (1-x)(a+b) \rfloor$ times and then uses

$$I_x(a,b) = x^a(1-x)^{b}\frac{\Gamma(a+b)}{\Gamma(a+1)\Gamma(b)} + I_x(a+1,b)$$

repeatedly until convergence is attained. For $x > a/(a+b)$ and $a, b \ge 1$ we first use $I_x(a,b) = 1 - I_{(1-x)}(b,a)$ and then apply the algorithm to $I_{(1-x)}(b,a)$. For either $a < 1$ or $b < 1$ we use

$$I_x(a,b) = x^a(1-x)^{b}\frac{\Gamma(a+b)}{\Gamma(a+1)\Gamma(b)}\left(1 - \frac{x(a+b)}{b}\right) + I_x(a+1,b+1)$$

and then apply the previous to $I_x(a+1,b+1)$.

The incomplete gamma c.d.f. is calculated using the series

$$G(x,a) = \frac{x^a e^{-x}}{\Gamma(a)}\sum_{k=0}^{\infty}\frac{x^k}{(a+k)_{k+1}}$$

for small x and using

$$G(x,a) = 1 - \frac{x^a e^{-x}}{\Gamma(a)}c(x)$$

where the continued fraction

$$c(x) = 1/\{x+(1-a)/\{1+1/\{x+(2-a)/\{1+2/\{x+\cdots(k-a)/\{1+k/\{x+\cdots\ .$$

for large x.

[1]Soper, H.E. (1921) The numerical evaluation of the incomplete beta function or of the integral $\int_0^x t^{p-1}(1-t)^{q-1}dt$ for ranges of x between 0 and 1. *Tracts for Computers No. VII*, edited by Karl Pearson. Cambridge University Press, Cambridge, England.

The hypergeometric c.d.f. is calculated with

$$F_X(x; N, D, n) = p(x; N, D, n) \left(1 + \sum_{k=1}^{x-L} \frac{(x)_k (N - D - n + x)_k}{(D - x + k)_k (n - x + k)_k} \right)$$

where $L = \max\{0, D + n - N\}$ and

$$p(x; N, D, n) = \binom{n}{x} \frac{(D)_x (N - D)_{n-x}}{(N)_n}$$

for $x \leq (D + 1)(n + 1)/(N + 2)$ the mode. For $x > (D + 1)(n + 1)/(N + 2)$ we use the identity

$$F_X(x; N, D, n) = 1 - F_X(D - x - 1; N, D, N - n)$$

and apply the sum to $F_X(D - x - 1; N, D, N - n)$.

3.2 Problems

1. Let $h(x)$ be a measurable function from R to R. That is for $\mathcal{B}$ the smallest sigma field generated by intervals in R, then $h^{-1}(B) \in \mathcal{B}$ for $B \in \mathcal{B}$. Prove that for X, a measurable random variable, $\mathcal{A}(Y) \subset \mathcal{A}(X)$ if $Y = h(X)$.

2. Prove that the negative binomial c.d.f. can be expressed in terms of the binomial c.d.f. by

$$F_Y(y; r, p) = \sum_{k=0}^{y} \binom{r + k - 1}{k} p^r q^k =$$

$$\sum_{k=r}^{y+r} \binom{y + r}{k} p^k q^{y+r-k} = 1 - F_X(r - 1; y + r, p) \ .$$

3 Prove that for the binomial c.d.f. we have

$$F_X(x; n, p) = 1 - F_X(n - x - 1; n, q) \ .$$

4. Prove for the hypergeometric c.d.f.

$$F_X(x; N, D, n) = F_X(x; N, n, D) = 1 - F_X(n - x - 1; N, N - D, n) \ .$$

5. Show for the negative binomial p.d.f. that

$$\binom{r+y-1}{y} p^r q^y \longrightarrow \frac{\lambda^y}{y!} e^{-\lambda}$$

as $r \to \infty$ and $rq \to \lambda > 0$.

6. Show for the hypergeometric p.d.f.

$$\binom{n}{x} \frac{(D)_x (N-D)_{n-x}}{(N)_n} \longrightarrow \binom{n}{x} p^x q^{n-x}$$

as $N \to \infty$ and $D/N \to p$, $0 < q = 1 - p < 1$

7. Calculate $F_X(20; 49, 0.48)$ for the binomial c.d.f.

8. Calculate $F_Y(20; 10, 0.37)$ for the negative binomial c.d.f.

9. Calculate $F_X(250; 1000, 500, 500)$ for the hypergeometric c.d.f.

10. Calculate $F_Y(245; 1000, 500, 250)$ for the negative hypergeometric c.d.f.

11. Calculate $F_X(9; 10)$ for the Poisson c.d.f.

Chapter 4

Continuous Distributions

Previously we have considered discrete random variables that can only take on a finite or countably infinite number of values. We now consider random variables that take on a continuum of values such as in an interval on the real line. Distributions for such random variables are often obtained as limits of discrete random variables.

To illustrate, consider a sequence of discrete random variables $\{X_n \,:\, n = 1, 2, \ldots\}$ where

$$P(X_n = k/n) = \frac{2}{n-1}\left(1 - \frac{k}{n}\right) \text{ for } k = 1, 2, \ldots, n.$$

This is a triangular shaped discrete density with c.d.f.

$$\sum_{k\,:\,k/n \le x} \frac{2}{n-1}\left(1 - \frac{k}{n}\right) = \sum_{k \le \lfloor nx \rfloor} \frac{2}{n-1}\left(1 - \frac{k}{n}\right) \longrightarrow x(2-x) \text{ for } 0 < x \le 1$$

since for $r = \lfloor nx \rfloor$ we have $r/n \to x$ and $\sum_{k=1}^{r} k = r(r+1)/2$ and $r(r+1)/(n(n-1)) \to x^2$ as $n \to \infty$.

This c.d.f. limit takes values in the interval $(0, 1]$ and can be viewed as the area under the function $f(x) = 2(1-x)$ from 0 to $x \le 1$. Note that the probability of any value approaches zero but that the probability for an interval goes to the area under the function over that interval. If we define $X = \lim_{n\to\infty} X_n$ as a random variable with the c.d.f. $x(2-x)$, it is a continuous random variable with continuous probability density $f_X(x) = 2(1-x)$ for $0 < x \le 1$. The pictures are as follows for the discrete density with $n = 20$ and the limiting function $f(x)$. Bars centered at each $x = k/n$ are used here instead of lines for the p.d.f. plot.

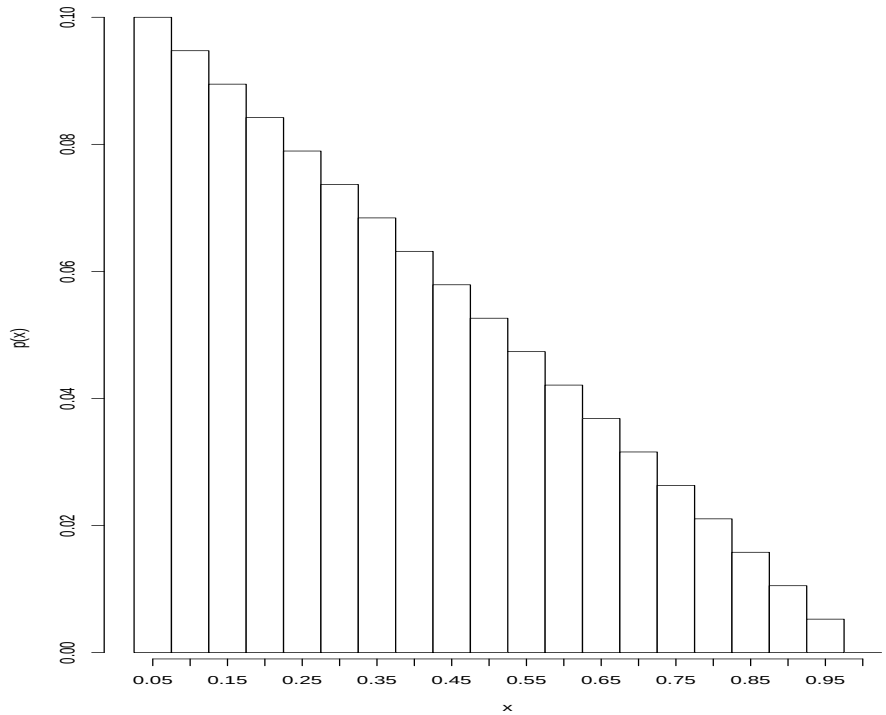

Figure 4.1: Discrete density $f_{X_n}(x) = 2(1-x)/(n-1)$ for $x = 1/n, 2/n, \ldots, n/n = 1, \quad n = 20$.

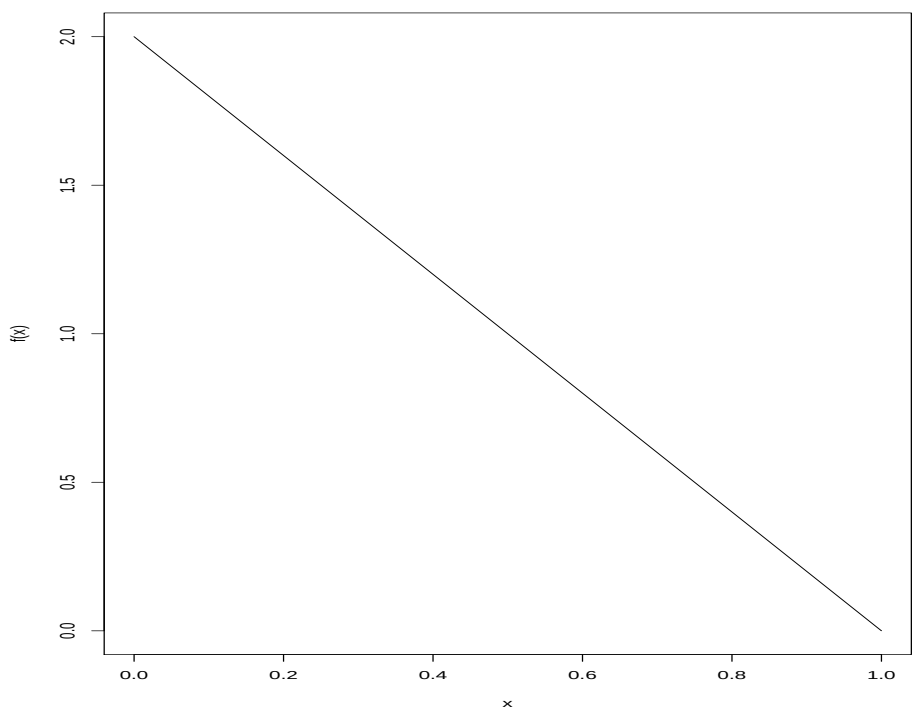

Figure 4.2: Limiting continuous density $f(x) = 2(1-x)$ for $0 < x \leq 1$.

In general, we can define a continuous random variable by assigning a function $f_X(x)$ that is called a continuous density function. It is used to spread the unit of probability over the real line and has the properties

$$f_X(x) \geq 0 \text{ and } \int_{-\infty}^{\infty} f_X(x)dx = 1 \ .$$

Thus it is a nonnegative function that has area 1 and

$$P(a < X \leq b) = \int_a^b f_X(x)dx \ .$$

The continuous density function is not a probability. It must be integrated to find the area over a set to get the set's probability. The expected value for a random variable with a continuous density is

$$E(g(X)) = \int_{-\infty}^{\infty} g(x)f_X(x)dx \ .$$

Some properties are

$$\begin{aligned} E(g(X) + t(X)) &= E(g(X)) + E(t(X)) \\ E(aX + b) &= aE(X) + b \\ E(C) &= C \end{aligned}$$

4.1 Continuous Density Examples

There are many examples of continuous densities. Some commonly used ones are:

The standard normal density $f_X(x) = e^{-x^2/2}/\sqrt{2\pi}$ for $-\infty < x < \infty$ often refered to as the $\mathcal{N}(0,1)$ density.Figure 4.3 plots the density. The area between the two vertical lines under the density gives $P(-1 < X < 2)$

The general normal density with parameters $-\infty < \mu < \infty$, $\sigma > 0$ given by

$$f_X(x) = \frac{e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}}{\sigma\sqrt{2\pi}}$$

for $-\infty < x < \infty$. It is called the $\mathcal{N}(\mu, \sigma^2)$ density.

The standard Cauchy density or Cauchy with location and scale parameters $-\infty < \mu < \infty$, $\sigma > 0$ for $-\infty < x < \infty$

$$f_X(x) = \frac{1}{\pi(1+x^2)}, \quad f_X(x) = \frac{1}{\sigma\pi\left(1+\left(\frac{x-\mu}{\sigma}\right)^2\right)} .$$

The standard exponental density and exponential density with location and scale parameters $-\infty < \mu < \infty$, $\sigma > 0$

$$f_X(x) = \begin{cases} e^{-x} & \text{for } 0 \le x < \infty \\ 0 & \text{for } x < 0. \end{cases}, \quad f_X(x) = \begin{cases} \frac{1}{\sigma}e^{-(x-\mu)/\sigma} & \text{for } \mu \le x < \infty \\ 0 & \text{for } x < \mu. \end{cases}$$

The gamma density with shape and scale parameters $\alpha, \sigma > 0$

$$f_X(x) = \frac{x^{\alpha-1}e^{-x/\sigma}}{\sigma^\alpha\Gamma(\alpha)}, \text{ for } x > 0, \text{ and } f_X(x) = 0, \text{ for } x \le 0.$$

The chi-square density χ^2_n with density

$$f_X(x) = \frac{x^{n/2-1}e^{-x/2}}{\Gamma(n/2)2^{n/2}} \text{ for } 0 < x\infty$$

is a special case of the gamma with $\alpha = n/2$ and $\sigma = 2$.

The beta density with shape parameters $\alpha, \beta > 0$

$$f_X(x) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}x^{\alpha-1}(1-x)^{\beta-1} \text{ for } 0 < x < 1, \text{ and } f_X(x) = 0 \text{ elsewhere.}$$

The Weibull density with parameters $\beta, \sigma > 0$

$$f_X(x) = \frac{\beta}{\sigma^\beta}x^{\beta-1}e^{-(x/\sigma)^\beta} \text{ for } x > 0, \text{ and } f_X(x) = 0, \text{ for } x \le 0.$$

The double exponential with parameters $-\infty < \mu < \infty$, $\sigma > 0$

$$f_X(x) = \frac{1}{2\sigma}e^{-|x-\mu|/\sigma} \text{ for } -\infty < x < \infty.$$

4.1.1 C.D.F. for Continuous random Variables

The c.d.f. for a continuous random variable is

$$F_X(x) = P(-\infty < X \leq x) = \int_{-\infty}^{x} f_X(u)du \ .$$

To calculate $P(a < X \leq b) = P(a \leq X < b) = P(a < X < b) = P(a \leq X \leq b)$ which are all the same for a continuous random variable since the probability of a single point is zero, we can use $F_X(b) - F_X(a)$.

For the standard normal $\mathcal{N}(0,1)$ density, the c.d.f. function is often denoted by $\Phi(x)$. For general normal $\mathcal{N}(\mu, \sigma^2)$ random variables we can express the c.d.f. in terms of $\Phi(z)$ as

$$F_X(x) = \Phi((x-\mu)/\sigma) \ .$$

For a density symmetric about 0 we have $F_X(-x) = (1 - F_X(x))$. We note this holds for the $\mathcal{N}(0,1)$ c.d.f. ($\Phi(-x) = (1 - \Phi(x))$).

Appendix B gives the C++ subroutine **normal.h** for the $\mathcal{N}(0,1)$ c.d.f.

For small x we use the series

$$\Phi(x) = \frac{1}{2} + \frac{xe^{-x^2/2}}{\sqrt{2\pi}} \sum_{k=0}^{\infty} \frac{x^{2k}}{1 \times 3 \times \cdots (2k+1)} \ .$$

For large positive or negative x we use the continued fraction

$$c(x) = 1/\{x + 1/\{x + 2/\{x + 3/\{x + \cdots k/\{x + \cdots$$

with

$$\Phi(x) = \begin{cases} 1 - \frac{e^{-x^2/2}}{\sqrt{2\pi}} c(x) & \text{for } x > 0 \\ -\frac{e^{-x^2/2}}{\sqrt{2\pi}} c(x) & \text{for } x < 0 \end{cases}$$

4.2 Problems

1. For the standard normal $\mathcal{N}(0,1)$ random variable, caculate $P(-1 < X < 2)$ to 12 decimals.

2. For the gamma density with $\alpha = 3$ and $\sigma = 2$, calculate $P(5 < X < 8)$.

3. For the beta density with $\alpha = 3$ and $\beta = 7$ calculate $P(0.15 < X < 0.6)$.

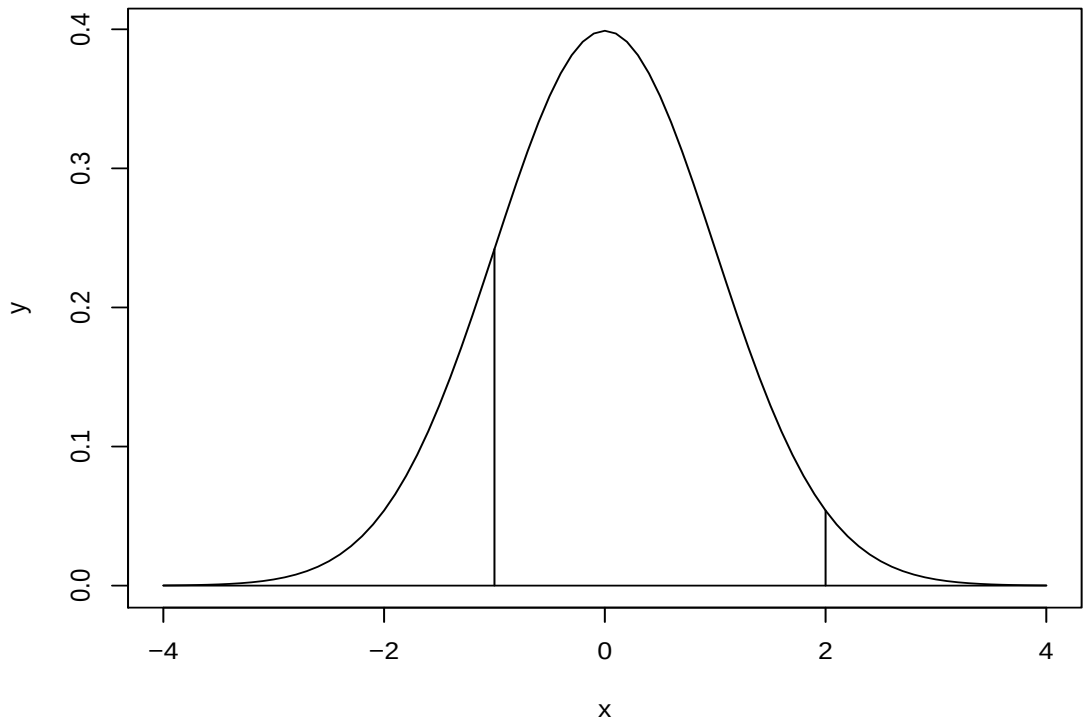

Figure 4.3: Normal $\mathcal{N}(0,1)$ density showing area between vertical lines for $P(-1 < X < 2)$.

Chapter 5

The General Case

5.1 Some Measure Theory

5.1.1 Measure Definition

A measure μ is a set function defined on a sample space and sigma field $(\Omega, \mathcal{A})$ that satisfies

(i) $\mu(A) \geq 0$ for $A \in \mathcal{A}$.

(ii) If $\{A_i : i = 1, 2, \ldots, \infty\}$ is an infinite collection of disjoint sets ($A_i \cap A_j = \phi$ for $i \neq j$) then $\mu(\bigcup_{i=1}^{\infty} A_i) = \sum_{i=1}^{\infty} \mu(A_i)$.

We say the measure μ is sigma finite if we can find a disjoint partition of the sample space $\Omega = \bigcup_{i=1}^{\infty} A_i$ such that $\mu(A_i) < \infty$ for all $i = 1, 2, \ldots, \infty$.

An important example is *counting measure* on R^n. Here Ω is a set of vectors in R^n with integer components $\mathcal{A}$ is the sigma field of all subsets of Ω, and $\mu(A)$ is the count of the number of such vectors in A.

Another important example is *Lebesgue measure*. Here Ω is the n dimensional Euclidean space $R^n = \{(x_1, x_2, \ldots, x_n) : -\infty < x_i < \infty\}$, $\mathcal{A} = \mathcal{B}^{(n)}$ is the Borel sigma field on R^n which is the smallest sigma field that contains all rectangles $A = \{(x_1, x_2, \ldots, x_n) : a_i < x_i < b_i\}$ for all $a_i < b_i$. Then the measure μ is determined from the value for rectangles $\mu(A) = \prod_{i=1}^{n}(b_i - a_i)$.

Theorem 5.1 *If $A_n \in \mathcal{A}$, $A_n \uparrow A$ then $\mu(A_n) \to \mu(A)$.*

Proof.
If $\mu(A_n) = \infty$ for some n, then

$$\mu(A) = \mu(A_n) + \mu(A \cap A_n^c) = \infty \ .$$

Thus $\mu(A_k) = \infty$ for $k \geq n$ so $\lim_n \mu(A_n) = \infty = \mu(A)$.

Next assume $\mu(A_n) < \infty$ for all n.

$$A = A_1 \cup \bigcup_{i=2}^{\infty} (A_i \cap A_{i-1}^c)$$

and using additivity for disjoint events and $\mu(A_i) = \mu(A_{i-1}) + \mu(A_i \cap A_{i-1}^c)$ for $A_{i-1} \subset A_i$

$$\mu(A) = \mu(A_1) + \sum_{i=2}^{\infty} (\mu(A_i) - \mu(A_{i-1})) = \lim_n \mu(A_n) \,. \blacksquare$$

5.1.2 Definition of the Integral of a Function

Define an indicator function for an event A by

$$I_A(x) = \begin{cases} 1 & \text{if } x \in A \\ 0 & \text{if } x \notin A \,. \end{cases}$$

Next define a simple function (a function that takes a finite number of values) for $\Omega = \bigcup_{i=1}^k A_i$, where $A_i \in \mathcal{A}$ are disjoint, by

$$h(x) = \sum_{i=1}^{k} a_i I_{A_i}(x) \quad \text{so that } h(x) = a_i \text{ for } x \in A_i \,.$$

Then for this simple function we define

$$\int_\Omega h(x) d\mu(x) = \sum_{i=1}^{k} a_i \mu(A_i)$$

Next, for measurable $h(x) \geq 0$ define

$$\int_\Omega h(x) d\mu(x) = \sup\{\int_\Omega s(x) d\mu(x) : s \text{ simple}, 0 \leq s(x) \leq h(x)\}$$

Finally, for measurable $h(x)$ define

$$\int_\Omega h(x) d\mu(x) = \int_\Omega h_+(x) d\mu(x) - \int_\Omega h_-(x) d\mu(x)$$

where $h_+(x) = \max\{0, h(x)\} \geq 0$ and $h_-(x) = \max\{0, -h(x)) \geq 0$. The integral is well defined and for Lebesgue measure it equals the more commonly used Rieman integral when the Rieman integral exists. For counting measure, it reduces to a sum.

Theorem 5.2 Jensen's Inequality. *If $h(x)$ is a continuous function defined on an open interval $I = (a, b)$ and convex*

$$h(\lambda x + (1-\lambda)y) \leq \lambda h(x) + (1-\lambda)h(y)$$

for $0 < \lambda < 1$, $a < x < y < b$), and $P(X \in (a, b)) = 1$, then

$$h(E(X)) \leq E(h(X)) \ .$$

For a proof see, for example, Ash[1].

Theorem 5.3 *Let $h \geq 0$ be measurable and define*

$$\lambda(B) = \int_B h(x) d\mu(x) \ .$$

Then λ is a measure.

Proof.
Let h be a nonnegative simple function. Then

$$\lambda(B) = \int_B h(x) d\mu(x) = \sum_{i=1}^{k} x_i \mu(B \cap A_i)$$

and since μ is countably additive and $h \geq 0$ gives $\lambda(B) \geq 0$ it is a measure.

Next let h be a nonnegative measurable function.
For simple s, $0 \leq s \leq h$ and $B = \bigcup_{i=1}^{\infty} B_n$ where $B_n \in \mathcal{A}$ are disjoint

$$\int_B s(x) d\mu(x) = \sum_{i=1}^{\infty} \int_{B_n} s(x) d\mu(x)$$

[1] Ash, Robert B. (1972) *Real Analysis and Probability.* Academic Press, Inc. Harcourt Brace Janovich Publishers, San Diego, California. pp. 286-288.

since the previous proved the integral a measure for a simple function and it has countable additivity. In turn

$$\int_B s(x)d\mu(x) \leq \sum_{i=1}^{\infty} \sup\{\int_{B_n} s(x)d\mu(x) : s \text{ simple}, 0 \leq s \leq h\}$$

$$= \sum_{i=1}^{\infty} \int_{B_n} h(x)d\mu(x) = \sum_{i=1}^{\infty} \lambda(B_n)$$

Taking the sup of $\int_B s(x)d\mu(x)$ gives $\lambda(B) \leq \sum_{i=1}^{\infty} \lambda(B_n)$.

To finally show $\lambda(B) \geq \sum_{i=1}^{\infty} \lambda(B_n)$.

We have $B_n \subset B$ so that $I_{B_n} \leq I_B$ and $\lambda(B_n) \leq \lambda(B)$ which follows from the definition of the integral. If $\lambda(B_n) = \infty$ for some n equality holds trivially. Assume $\lambda(B_n) < \infty$ for all n. We can find a simple function s with $0 \leq s \leq h$ such that

$$\int_{B_k} s(x)d\mu(x) \geq \int_{B_k} h(x)d\mu(x) - \frac{\varepsilon}{n} \text{ for } k = 1, 2, \ldots, n \ .$$

Then

$$\lambda(\bigcup_{k=1}^{n} B_k) = \int_{\bigcup_{k=1}^{n} B_k} h(x)d\mu(x) \geq \int_{\bigcup_{k=1}^{n} B_k} s(x)d\mu(x)$$

$$= \sum_{k=1}^{n} \int_{B_k} s(x)d\mu(x) \geq \sum_{k=1}^{n} \int_{B_k} h(x)d\mu(x) - \varepsilon = \sum_{k=1}^{n} \lambda(B_k) - \varepsilon$$

Thus letting $\varepsilon \downarrow 0$

$$\lambda(B) \geq \lambda(\bigcup_{k=1}^{n} B_k) \geq \sum_{k=1}^{n} \lambda(B_k) \ .$$

Letting $n \to \infty$ we have $\lambda(B) \geq \sum_{i=1}^{\infty} \lambda(B_n)$.■

Also convergence theorems are valid such as the monotone convergence theorem and the dominated convergence theorem.

Theorem 5.4 Monotone Convergence Theorem. *Let h_n be measurable, $0 \leq h_n \uparrow h$. Then*

$$\int_\Omega h_n(x)d\mu(x) \longrightarrow \int_\Omega h(x)d\mu(x) \ .$$

Proof.

$$0 \le h_n \le h \Longrightarrow \int_\Omega h_n(x)d\mu(x) \le \int_\Omega h(x)d\mu(x)$$

and

$$K = \lim_n \int_\Omega h_n(x)d\mu(x) \le \int_\Omega h(x)d\mu(x) \ .$$

Next, let $0 < b < 1$ and let s be a non negative simple function with $s \le h$. Define

$$B_n = \{x : h_n(x) \ge bs(x)\} \uparrow \Omega$$

since $h_n \uparrow h$ and s is finite valued. We have

$$K \ge \int_\Omega h_n(x)d\mu(x) \ge \int_{B_n} h_n(x)d\mu(x) \le \int_\Omega h(x)d\mu(x) \ge b\int_{B_n} s(x)d\mu(x) \ .$$

Now $\lambda(B_n) = \int_{B_n} s(x)d\mu(x)$ is a measure and so $\lambda(B_n) \to \lambda(\Omega)$ and

$$K \ge b\int_\Omega s(x)d\mu(x) \ .$$

Letting $b \uparrow 1$ and taking the sup of the integral for simple s, $0 \le s \le h$ gives

$$K \ge \int_\Omega h(x)d\mu(x) \ . \blacksquare$$

Define

$$\liminf_{n\to\infty} f_n(x) = \sup_n \inf_{k\ge n} f_k(x), \quad \limsup_{n\to\infty} f_n(x) = \inf_n \sup_{k\ge n} f_k(x) \ .$$

We have the following:

Lemma 5.1 Fatou's Lemma. *Let $f_1, f_2, \ldots, f$ be measurable functions.*
(a) If $f_n \ge f$ for all n where $\int_\Omega f(x)d\mu(x) > -\infty$, then

$$\liminf_{n\to\infty} \int_\Omega f_n(x)d\mu(x) \ge \int_\Omega \left(\liminf_{n\to\infty} f_n(x)\right) d\mu(x) \ .$$

(b) If $f_n \le f$ for all n where $\int_\Omega f(x)d\mu(x) < \infty$, then

$$\limsup_{n\to\infty} \int_\Omega f_n(x)d\mu(x) \le \int_\Omega \left(\limsup_{n\to\infty} f_n(x)\right) d\mu(x) \ .$$

Proof.
(a) Let $g_n = \inf_{k\geq n} f_k$ and $g = \liminf_n f_n$. Then $g_n \geq f$ for all n, and $g_n \uparrow g$. Thus by the monotone convergence theorem applied to $0 \leq (g_n - f) \uparrow (g - f)$,

$$\int_\Omega g_n(x)d\mu(x) \longrightarrow \int_\Omega (\liminf_n f_n(x))d\mu(x) \ .$$

Since $g_n \leq f_n$

$$\int_\Omega (\liminf_n f_n(x))d\mu(x) = \lim_n \int_\Omega g_n(x)d\mu(x)$$

$$= \liminf_n \int_\Omega g_n(x)d\mu(x) \leq \liminf_n \int_\Omega f_n(x)d\mu(x) \ .$$

(b) Since $\limsup_n f_n = -\liminf_n(-f_n)$ we can use (a)

$$\int_\Omega \limsup_n f_n(x)d\mu(x) = -\int_\Omega \liminf_n(-f_n(x)d\mu(x)$$

$$\geq -\liminf_n \int_\Omega (-f_n(x))d\mu(x) = \limsup_n \int_\Omega f_n(x)d\mu(x) \ .\blacksquare$$

Theorem 5.5 Dominated Convergence Theorem.

$$\int_\Omega f_n(x)d\mu(x) \longrightarrow \int_\Omega f(x)d\mu(x)$$

provided $f_n(x) \to f(x)$ *and* $|f_n(x)| \leq g(x)$ *as* $n \to \infty$ *where*

$$\int_\Omega g(x)d\mu(x) < \infty \ .$$

Proof.
Using Fatou's lemma, since $-g(x) \leq f_n(x) \leq g(x)$, $\int_\Omega(-g(x))d\mu(x) > -\infty$, and $\int_\Omega g(x)d\mu(x) < \infty$,

$$\int_\Omega \liminf_n f_n(x)d\mu(x) \leq \liminf_n \int_\Omega f_n(x)d\mu(x)$$

$$\leq \limsup_n \int_\Omega f_n(x)d\mu(x) \leq \int_\Omega \limsup_n f_n(x)d\mu(x) \ .$$

But $f = \lim_n f_n = \liminf_n f_n = \limsup_n f_n$ so

$$\lim_n \int_\Omega f_n(x)d\mu(x) = \int_\Omega f(x)d\mu(x).\blacksquare$$

5.1.3 Derivatives for Measures

We say a measure ν is absolutely continuous with respect to the measure μ and write $\nu << \mu$ if $\mu(A) = 0$ implies $\nu(A) = 0$ for $A \in \mathcal{A}$.

The following Radon-Nikodym theorem is proved in courses on measure theory. See, for example, Ash (1972)[2].

Theorem 5.6 Radon-Nikodym Theorem. *Let μ and ν be sigma finite measures. Then there exists a nonnegative $\mathcal{A}$ measurable function f such that*

$$\nu(A) = \int_A f(x)d\mu(x) = \int_\Omega I_A(x)f(x)d\mu(x) \ .$$

if and only if ν is absolutely continuous with respect to μ ($\nu << \mu$). If g is another function satisfying the above equations, then $g = f$ a.e. $[\mu]$.

The function $f(x)$ is often denoted

$$f(x) = \frac{d\nu}{d\mu}(x) \ .$$

Theorem 5.7 Chain Rule. *If $\eta << \nu << \mu$ then*

$$\frac{d\eta}{d\mu} = \frac{d\eta}{d\nu}\frac{d\nu}{d\mu} \ .$$

Proof
We first prove that if $\eta(A) = \int_A f(x)d\nu(x)$ and $\nu(A) = \int_A g(x)d\mu(x)$ then

$$\int_\Omega f(x)d\nu(x) = \int_\Omega f(x)g(x)d\mu(x) \ .$$

If $f(x) = \sum_{i=1}^k x_i I_{A_i}(x)$ is simple, then

$$\int_\Omega f(x)d\nu(x) = \sum_{i=1}^k x_i\nu(A_i) = \sum_{i=1}^k x_i \int_{A_i} g(x)d\mu(x)$$

$$= \int_\Omega \sum_{i=1}^k x_i I_{A_i}(x)g(x)d\mu(x) = \int_\Omega f(x)g(x)d\mu(x) \ .$$

[2]Robert B. Ash (1972). *Real Analysis and Probability.* Academic Press, Inc. Harcourt Brace Janovich, Publishers. San Diego, California. pp. 63-65.

Next, if $f \geq 0$ is measurable, let $f_n \uparrow f$ where f_n is simple. Then

$$\int_\Omega f_n(x)d\nu(x) = \int_\Omega f_n(x)g(x)d\mu(x)$$

and using the monotone convergence theorem, $n \to \infty$,

$$\int_\Omega f(x)d\nu(x) = \int_\Omega f(x)g(x)d\mu(x) \ .$$

Now let

$$\eta(A) = \int_\Omega I_A(x)f(x)d\nu(x), \text{ and } \nu(A) = \int_\Omega I_A(x)g(x)d\mu(x)$$

by the Radon-Nikodym theorem where $f = d\eta/d\nu$, $g = d\nu/d\mu$ since $\eta << \nu$ and $\nu << \mu$. Then by the above result

$$\eta(A) = \int_\Omega I_A(x)f(x)g(x)d\mu(x)$$

and

$$\frac{d\eta}{d\mu} = \frac{d\eta}{d\nu}\frac{d\nu}{d\mu} \ . \blacksquare$$

5.2 General Densities

Throughout, we will use $f_X(x)$ as the density of a random variable with respect to either counting measure for the discrete case or Lebesgue measure for the continuous case. We will write

$$P(X \in A) = \int_{x \in A} f_X(x)d\mu(x)$$

where μ is either counting measure (discrete case) or Lebesgue measure (continuous case) since $(\mu(A) = 0) \implies (P(X \in A) = 0)$ or $P_X << \mu$ for the discrete or continuous case.

5.2.1 Conditional Expectation

To define $E(h(X)|T(X))$ we first recall the sigma field $\mathcal{A}(T(X)) = \{A : A = T^{-1}(B), B \in \mathcal{B}\}$ for a measurable function $T(X)$. It is the class

of all sets that are inverse images under T of Borel sets. It is a subset of $\mathcal{A}$ since T is a measurable function.

Now we define $E(h(X)|T(X))$ as an $\mathcal{A}(T(X))$ measurable function that satisfies

$$\int_{A_0} h(x)f_X(x)d\mu(x) = \int_{A_0} E(h(X)|T(x))f_X(x)d\mu(x) \text{ for all } A_0 \in \mathcal{A}(T(X)) \ .$$

This definition uses the Radon-Nikodym theorem since

$$\nu(A_0) = \int_{A_0} h(x)f_X(x)d\mu(x) << \int_{A_0} f_X(x)d\mu(x) \text{ for } \mathcal{A}(T(X)) \ .$$

The $\mathcal{A}(T(X))$ measurable function that exists by the Radon-Nikodym theorem is called the conditional expectation $E(h(X)|T(X))$.

By setting $A_0 = \Omega$ in the definition we have

$$E(E(h(X)|T(X)) = E(h(X)) \ .$$

We also have the following properties:

If $Y = k$ a constant, a.e., then $E(Y|T(X)) = k$ a.e..

If $Y_1 \leq Y_2$ a.e., then $E(Y_1|T(X)) \leq E(Y_2|T(X))$ a.e..

$|E(Y|T(X))| \leq E(|Y||T(X))$.

$E(aY_1 + bY_2|T(X)) = aE(Y_1|T(X)) + bE(Y_2|T(X))$.

If $0 \leq Y_n \uparrow Y$ a.e., then $E(Y_n|T(X) \uparrow E(Y|T(X))$.

If $|Y_n| \leq g(X)$ with $E(g(X)) < \infty$ then $E(Y_n|T(X)) \to E(Y|T(X))$.

Chapter 6

Distribution Measures

There are various measures that help to describe the distribution of a random variable.

6.1 P.D.F. and C.D.F. Plots

The theoretical histogram or p.d.f. plot gives a visual display of the frequency of the various outcomes plotting $f_X(x)$ versus x.
Figure 6.1 gives the p.d.f. plot for the binomial with $n = 10$ and $p = 0.5$.
Figures 6.2, 6.3, 6.4, 6.5 give plots for the hypergeometric, negative binomial, Poisson, and negative hypergeometric.

A cumulative form of graphical display plots the c.d.f $F_X(x)$ versus x. For example the c.d.f. plot for the binomial with $n = 10$ and $p = 0.5$ is given in figure 6.6.

6.2 Measures of the Center

A theoretical *median* of the distribution is a number m for which
$P(X \leq m) \geq 1/2 \leq P(X \geq m)$. Such a number always exists.
For discrete random variables, if $F_X(x) = 1/2$ on an interval $a \leq x \leq b$ then any value m, $a \leq m \leq b$ can serve as a value for the median. The median can be read off the c.d.f. plot by looking at the horizontal line $y = 1/2$ and reading off the value(s) x where the line intersects the c.d.f. See the dotted line in figure 4.6.

Theorem 6.1 *The value of the constant C that minimizes $E|X-C|$ is $C=m$ where m is the median of the distribution of X.*

Proof.
Let $F_X(x)$ be the c.d.f. for X and write

$$E|X-C| = \int_{-\infty}^{\infty} |x-C| dF_X(x)$$

where we define the integral

$$\int_a^b h(x) dF_X(x) = \int_{(a,b]} h(x) f_X(x) d\mu(x)$$

$$= \begin{cases} \sum_{\substack{x: \\ a<x\le b}} h(x) f_X(x) & \text{for the discrete case} \\ \int_a^b h(x) f_X(x) dx & \text{for the continuous case, } f_X(x) = \frac{dF_X(x)}{dx} \ . \end{cases}$$

We note that the median m satisfies $F_X(m) \ge 1/2$ and $F_X(m-) \le 1/2$ where $F_X(m-) = \lim_{\varepsilon \downarrow 0} F_X(m-\varepsilon)$ since
$F_X(m) = P(X \le m) \ge 1/2 \le P(X \ge m) = 1 - P(X < m) = 1 - F_X(m-)$.
Then

$$\begin{aligned} E|X-C| - E|X-m| &= \int_{-\infty}^{C} (C-x) dF_X(x) + \int_C^{\infty} (x-C) dF_X(x) \\ &\quad - \int_{-\infty}^{m} (m-x) dF_X(x) - \int_m^{\infty} (x-m) dF_X(x) \\ &= \int_{-\infty}^{C} (C-m+m-x) dF_X(x) + \int_C^{\infty} (x-m+m-C) dF_X(x) \\ &\quad - \int_{-\infty}^{m} (m-x) dF_X(x) - \int_m^{\infty} (x-m) dF_X(x) \\ &= (C-m)(2F_X(C)-1) + 2\int_m^C (m-x) dF_X(x) \ . \end{aligned}$$

If $C \ge m$ then replacing x by C gives

$$\begin{aligned} E|X-C| - E|X-m| &\ge (C-m)(2F_X(C)-1) + 2(m-C)(F(C)-F(m)) \\ &= (C-m)(2F_X(m)-1) \ge 0 \ . \end{aligned}$$

If $C < m$ then replacing x by C for $x < m$ and noting $(x-m) = 0$ for $x = m$ gives

$$E|X - C| - E|X - m| \geq (m - C)(1 - 2F_X(C) + 2(m - C)(F(m-) - F(C))$$
$$= (m - C)(1 - 2F_X(m-)) \geq 0 \ . \blacksquare$$

Another measure of the center is the theoretical mean or expected value. It is often denoted by μ or $E(X)$ and, provided it is finite, it is defined by

$$E(X) = \int_{-\infty}^{\infty} x dF_X(x) \ .$$

It is the probability weighted sum of the values of the random variable in the discrete case and is the integral of the values multiplied by the continuous density in the continuous case. It is the center of balance of the p.d.f. plot in the discrete case and the center of balance of the continuous density in the continuous case.

Theorem 6.2 *The value of the constant C that minimizes $E(X - C)^2$ is $C = \mu = E(X)$.*

Proof.

$$E(X-C)^2 = E(X-\mu+\mu-C)^2 = E(X-\mu)^2 + 2(\mu-C)E(X-\mu) + (\mu-C)^2$$
$$= E(X - \mu)^2 + (\mu - C)^2 \geq E(X - \mu)^2 \ . \blacksquare$$

For the binomial we have

$$E(X) = \sum_{k=0}^{n} k \binom{n}{k} p^k q^{n-k} = np \ .$$

For the negative binomial

$$E(X) = \sum_{k=0}^{\infty} k \binom{r+k-1}{k} p^r q^k = \frac{rq}{p} \ .$$

For the Poisson

$$E(X) = \sum_{k=0}^{\infty} k \frac{\lambda^k}{k!} e^{-\lambda} = \lambda \ .$$

For the hypergeometric

$$E(X) = \sum_{k=L}^{U} k \begin{pmatrix} n \\ k \end{pmatrix} \frac{(D)_k (N-D)_{n-k}}{(N)_n} = \frac{nD}{N}$$

where $L = \max\{0, n+D-N\}$ and $U = \min\{n, D\}$.
For the negative hypergeometric

$$E(X) = \sum_{k=0}^{N-D} k \begin{pmatrix} r+k-1 \\ k \end{pmatrix} \frac{(D)_r (N-D)_k}{(N)_{r+k}} = \frac{r(N-D)}{(D+1)} \ .$$

For the $\mathcal{N}(\mu, \sigma^2)$ density, $E(X) = \mu$.
For the exponential(μ, σ) density , $E(X) = \mu + \sigma$.
For the gamma(α, σ) density, $E(X) = \alpha\sigma$.
For the beta(α, β) density , $E(X) = \alpha/(\alpha+\beta)$.
For the Weibull(β, σ) density , $E(X) = \sigma^{1/\beta}\Gamma(1+1/\beta)$.
For the double exponential(μ, σ) density, $E(X) = \mu$.

The derivation of the expectation of the binomial is

$$E(X) = \sum_{k=0}^{n} k \begin{pmatrix} n \\ k \end{pmatrix} p^k q^{n-k} = np \sum_{k=1}^{n} \begin{pmatrix} n-1 \\ k-1 \end{pmatrix} p^{k-1} q^{n-1-(k-1)}$$

$$= np \sum_{t=0}^{n-1} \begin{pmatrix} n-1 \\ t \end{pmatrix} p^t q^{n-1-t} = np(p+q)^{n-1} = np(1)^{n-1} = np \ . \blacksquare$$

The derivation for the $\mathcal{N}(\mu, \sigma^2)$ density is

$$E(X) = \int_{-\infty}^{\infty} x \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/(2\sigma^2)} dx$$

$$= \mu + \int_{-\infty}^{\infty} (x-\mu) \frac{1}{\sigma\sqrt{2\pi}} e^{-(x-\mu)^2/(2\sigma^2)} dx$$

$$= \mu + \sigma \int_{-\infty}^{\infty} t \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt = \mu \ . \blacksquare$$

Derivations for other expectations are similar and use the fact that the probability densities sum or integrate to one.

In general, the expectation of a function of a random variable is defined by

$$E(h(X)) = \int_{-\infty}^{\infty} h(x) dF_X(x).$$

provided that it is finite. Note $E(C) = C$ for a constant C since the probability density sums or integrates to 1.
An example with an infinite expectation is given by the p.d.f.

$$f_X(x) = \frac{6}{\pi^2 x^2} \text{ for } x = 1, 2, \ldots, \infty.$$

since the expectation is

$$E(X) = \sum_{x=1}^{\infty} x \frac{6}{\pi^2 x^2} = \frac{6}{\pi^2} \sum_{x=1}^{\infty} \frac{1}{x} = \infty \ .$$

6.3 Variance

A popular measure of spread of a distribution is the variance. It is often denoted by σ^2 or $\mathrm{Var}(X)$ and defined by

$$\mathrm{Var}(X) = E((X-\mu)^2) \text{ where } \mu = E(X) \ .$$

We have

$$E((X-\mu)^2) = E(X^2) - \mu^2$$

and also

$$= E(X(X-1)) - \mu(\mu-1) \ . \tag{6.1}$$

Proof.

$$E((X-\mu)^2) = E(X^2 - 2\mu X + \mu^2) = E(X^2) - 2\mu^2 + \mu^2 = E(X^2) - \mu^2 \ .$$

Also

$$E(X(X-1)) - \mu(\mu-1) = E(X^2 - X) - \mu^2 + \mu = E(X^2) - \mu - \mu^2 + \mu = E(X^2) - \mu^2 \ . \blacksquare$$

For $Y = aX + b$ we have $Var(Y) = a^2 Var(X)$.

Using equation (6.1) we can derive σ^2 for the various discrete distributions:

Binomial, $\sigma^2 = npq$,

Negative binomial, $\sigma^2 = rq/p^2$.

Poisson, $\sigma^2 = \lambda$.

Hypergeometric,

$$\sigma^2 = n\left(\frac{D}{N}\right)\left(\frac{N-D}{N}\right)\left(\frac{N-n}{N-1}\right) .$$

Negative hypergeometric,

$$\sigma^2 = \frac{r(N+1)(N-D)(D-r+1)}{(D+2)(D+1)^2} .$$

For the various continuous densities the variances are as follows:

$\mathcal{N}(\mu, \sigma^2)$ density $Var(X) = \sigma^2$.

Exponential(μ, σ) density $Var(X) = \sigma^2$.

Gamma(α, σ) density $Var(X) = \alpha\sigma^2$.

Beta(α, β) density $Var(X) = \alpha\beta/((\alpha+\beta)^2(\alpha+\beta+1))$.

Weibull(β, σ) density $Var(X) = \sigma^{2/\beta}(\Gamma(1+2/\beta) - \Gamma(1+1/\beta))$.

Double exponential(μ, σ) density $Var(X) = 2\sigma^2$.

The variance gives a bound on the probability outside an interval around the expectation.

Chebyshev's Theorem

For any constant $C > 1$

$$P(\mu - C\sigma < X < \mu + C\sigma) \geq 1 - \frac{1}{C^2}$$

where $\mu = E(X)$ and $\sigma^2 = Var(X)$.

Proof.

$$P(|X-\mu| \geq C\sigma) = \int_{\{|x-\mu|/(C\sigma)\geq 1\}} f_X(x)d\mu(x)$$
$$\leq \int_{-\infty}^{\infty} \frac{(x-\mu)^2}{C^2\sigma^2} f_X(x)d\mu(x) = \frac{1}{C^2} . \blacksquare$$

6.4 Problems

1. For the exponential distribution $f_X(x) = e^{-x/\sigma}/\sigma$ for $x > 0$ give the c.d.f. and the median.

2. For the geometric distribution $f_X(x) = q^x p$ where $p + q = 1$, $0 < p < 1$ and $x = 0, 1, 2, \ldots, \infty$, give the c.d.f. and the median.

3. For the Weibull(β, σ) distribution, give the c.d.f. and the median.

4. Derive the expectation and variance for the Poisson(λ) distribution.

5. Derive the expectation and variance for the negative binomial(r, p).

6. Derive the expectation and variance for the hypergeometric(N, D, n).

7. Derive the expectation and variance for the beta(α, β) distribution.

8. Derive the expectation and variance for the gamma(α, σ) distribution.

9 Derive the variance for the $\mathcal{N}(\mu, \sigma^2)$ distribution.

10 Derive the expectation and variance for the continuous uniform(a, b) density

$$f_X(x) = \frac{1}{(b-a)} \text{ for } a < x < b, \quad 0, \text{ otherwise.}$$

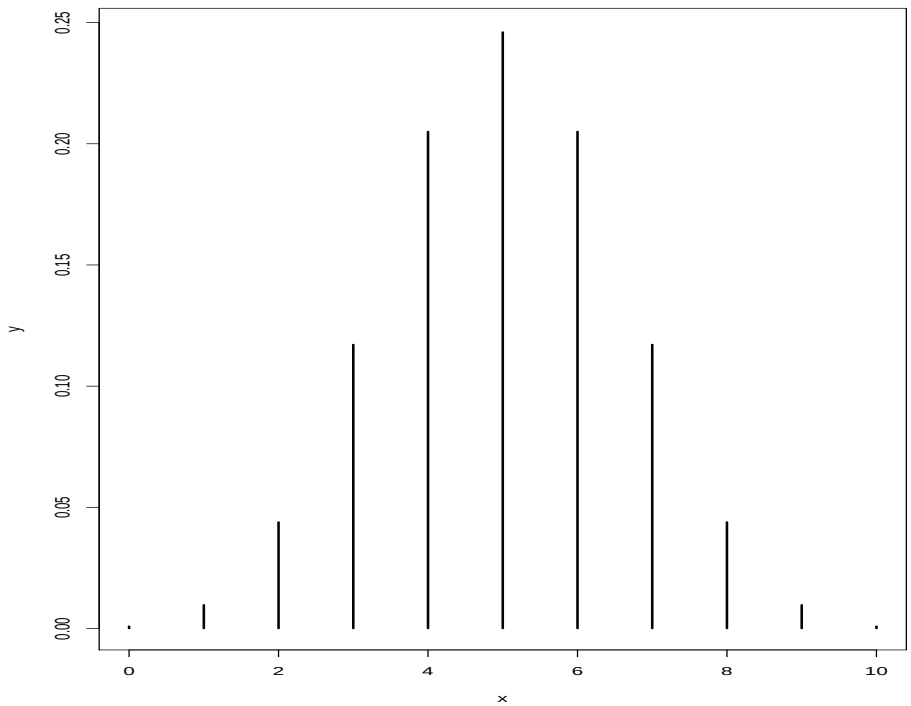

Figure 6.1: Binomial p.d.f. plot $(n, p) = (10, 0.5)$.

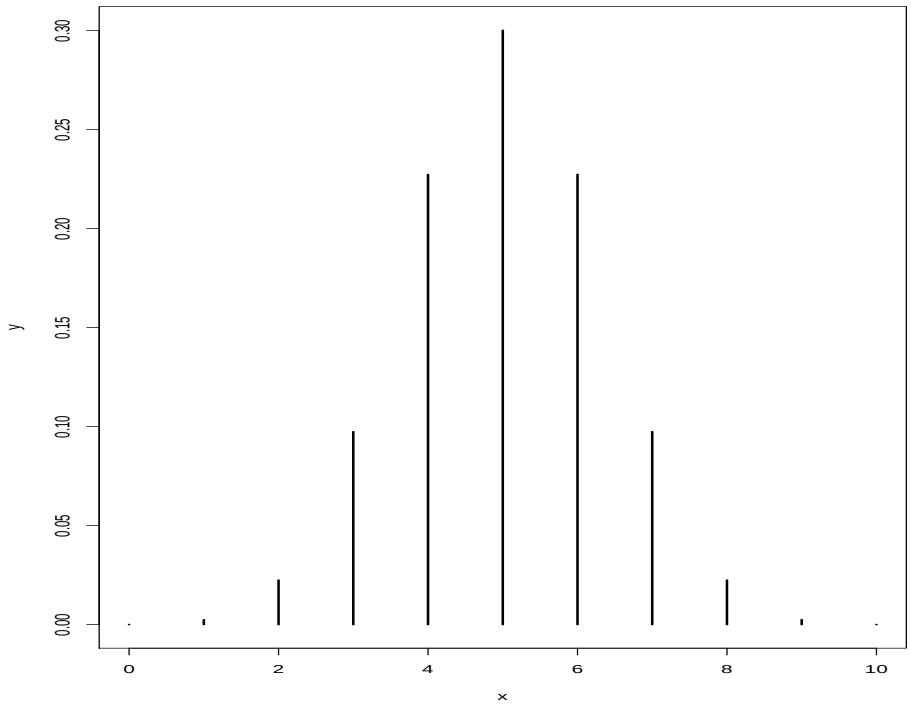

Figure 6.2: Hypergeometric p.d.f. plot $(N, D, n) = (30, 15, 10)$.

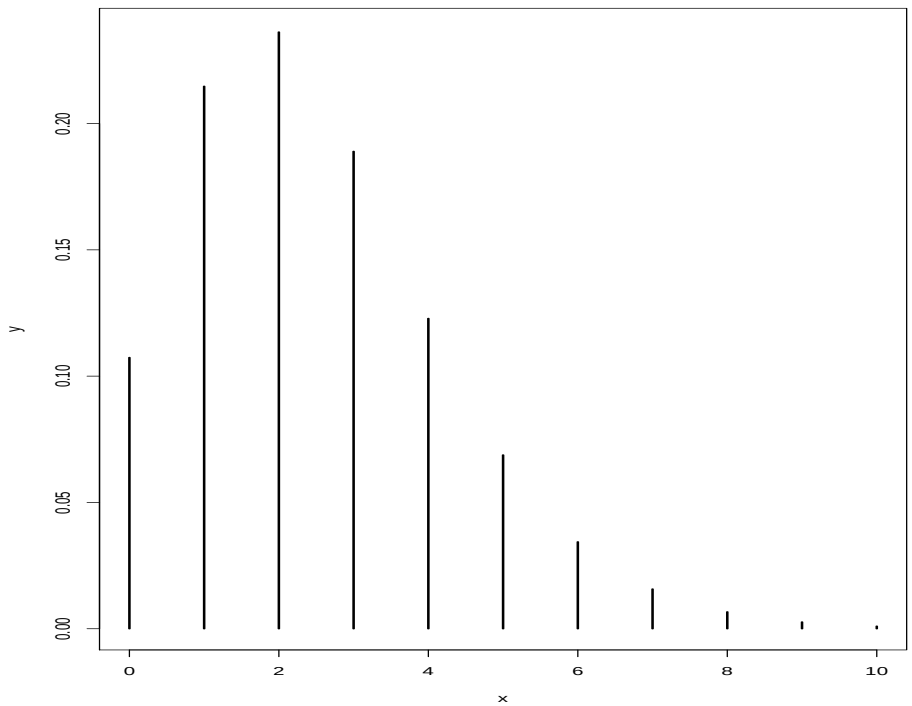

Figure 6.3: Negative binomial p.d.f. plot $(r, p) = (10, 0.8)$

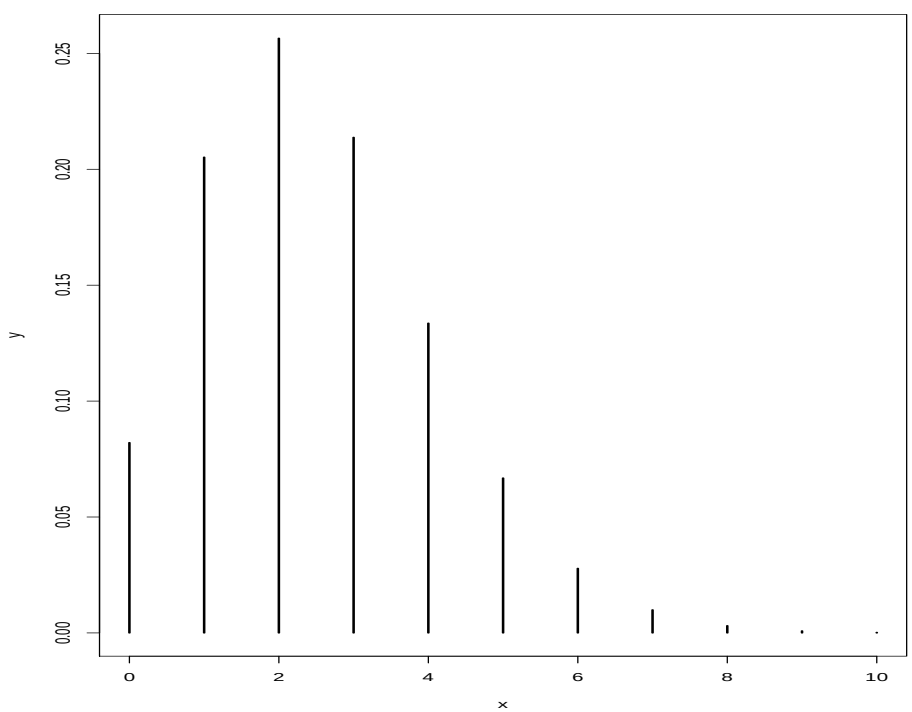

Figure 6.4: Poisson p.d.f. plot $\lambda = 2.5$.

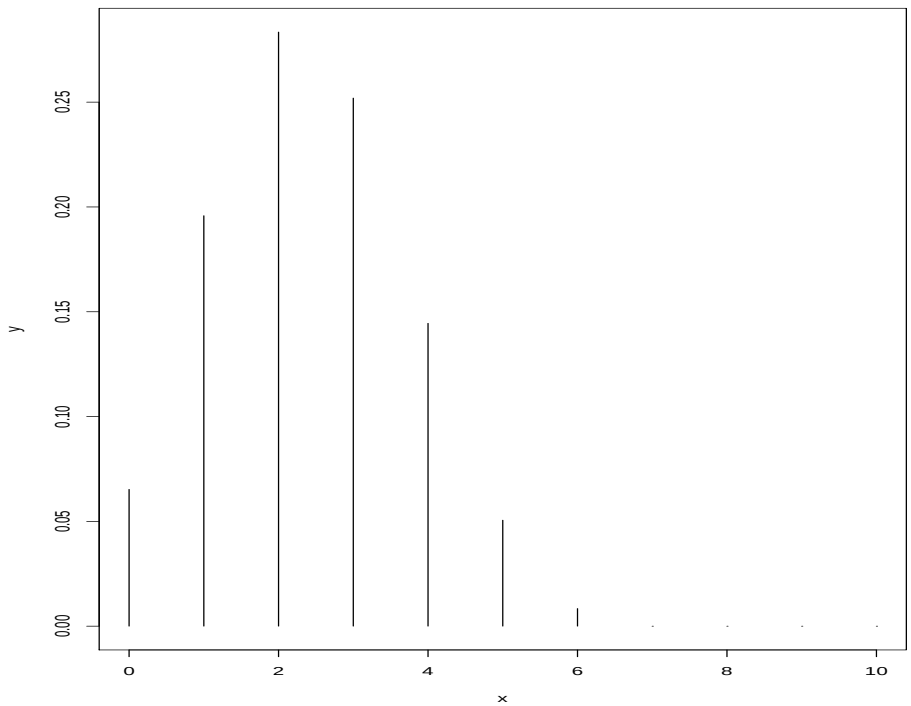

Figure 6.5: Negative hypergeometric p.d.f. plot $(N, D, r) = (30, 24, 10)$.

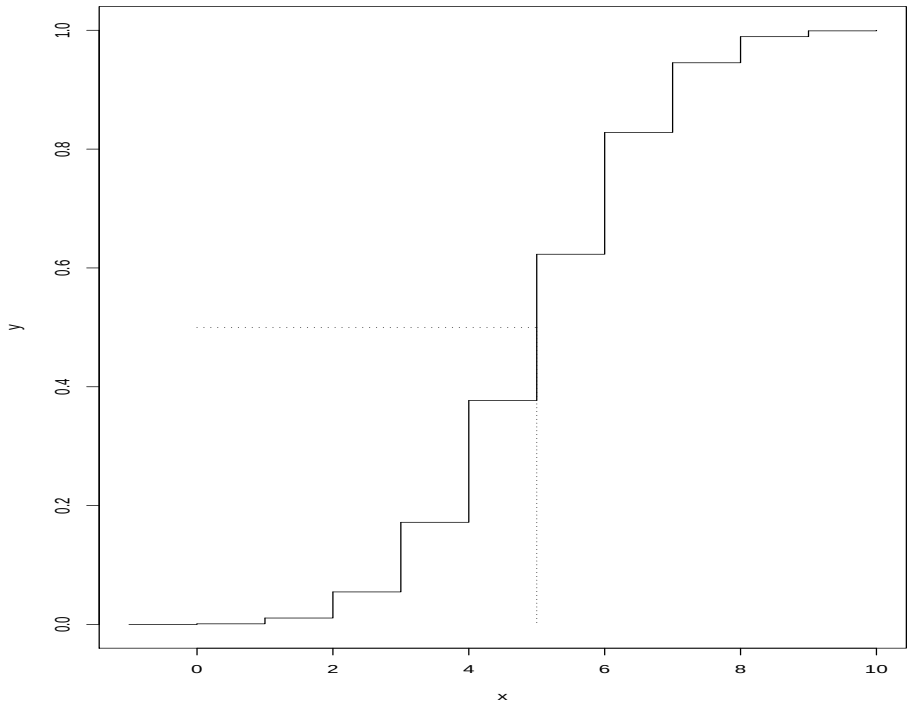

Figure 6.6: Binomial c.d.f. plot $(n, p) = (10, 0.5)$, median=5.

Chapter 7

Several Random Variables

7.1 Bivariate Random Variables

We define the distribution for two random variables X, Y in a manner similar to that for a single random variable.

$$P((X,Y) \in B^{(2)}) = P(A)$$

where

$$A = \{e \ : \ (X(e), Y(e)) \in B^{(2)}\} \text{ and } B^{(2)} \in \mathcal{B}^{(2)}$$

where $\mathcal{B}^{(2)}$ is the smallest sigma field generated by rectangles $(a_1, b_1] \otimes (a_2, b_2] = \{(x,y) \ : \ a_1 < x \leq b_1, \ a_2 < y \leq b_2\}$ in the plane.

For the discrete case where (X, Y) take on finite or countably infinite numbers of values the discrete joint density is

$$f_{X,Y}(x,y) = P(X = x, Y = y) \text{ where } \sum_{all\ x} \sum_{all\ y} f_{X,Y}(x,y) = 1 \ .$$

In the jointly continuous case we assign probabilities as the volume under the surface defined by a continuous 2 dimensional density $f_{X,Y}(x,y)$ and over the set $B^{(2)}$ in the (x,y) plane where the density satisfies

$$f_{X,Y}(x,y) \geq 0 \text{ and } \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f_{X,Y}(x,y) dx dy = 1 \ .$$

Thus the probability is the volume

$$P((X,Y) \in B^{(2)}) = \int \int_{\{(x,y) \in B^{(2)}\}} f_{X,Y}(x,y) dx dy \ .$$

For a discrete example, an urn contains R red, W white and B blue balls where $R+W+B=N$ total. A sample of n is selected without replacement and we observe X the number of red balls in the sample and Y the number of white balls in the sample. Then the bivariate hypergeometric p.d.f. is:

$$P(X=x,Y=y)=f_{X,Y}(x,y)=\frac{\begin{pmatrix} R \\ x \end{pmatrix}\begin{pmatrix} W \\ y \end{pmatrix}\begin{pmatrix} B \\ n-x-y \end{pmatrix}}{\begin{pmatrix} N \\ n \end{pmatrix}}$$

$$=\left(\frac{n!}{x!y!(n-x-y)!}\right)\frac{(R)_x(W)_y(B)_{(n-x-y)}}{(N)_n}\ .$$

Some important bivariate discrete densities are:

Trinomial(m,p_1,p_2,p_3):

$$f_{X,Y}(x,y)=\frac{m!}{x!y!(m-x-y)!}p_1^x p_2^y p_3^{m-x-y}$$

for $0<p_1,p_2,p_3<1$, $p_1+p_2+p_3=1$, and x,y,m integers, $0\le x,y\le m$, $x+y\le m$.

Bivariate hypergeometric(N,D_1,D_2,D_3,n)

$$f_{X,Y}(x,y)=\frac{\begin{pmatrix} D_1 \\ x \end{pmatrix}\begin{pmatrix} D_2 \\ y \end{pmatrix}\begin{pmatrix} D_3 \\ n-x-y \end{pmatrix}}{\begin{pmatrix} N \\ n \end{pmatrix}}$$

where D_1,D_2,D_3,N,n,x,y are integers, $D_1+D_2+D_3=N$.

Bivariate negative binomial(r,p_1,p_2,p_3):

$$f_{X,Y}(x,y)=\frac{(r+x+y-1)!}{x!y!(r-1)!}p_1^x p_2^y p_3^r$$

for $0<p_1,p_2,p_3<1$, $p_1+p_2+p_3=1$, and x,y,r integers.

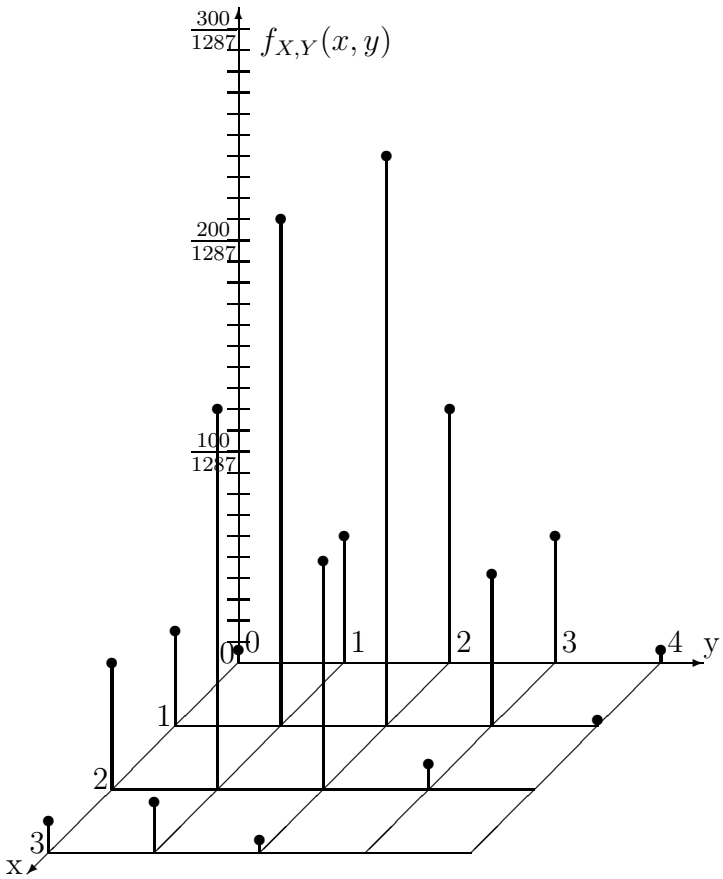

Figure 7.1: Plot of $f_{X,Y}(x,y)$ vs. (x,y) for bivariate hypergeometric disrtibution $(R,W,B) = (3,4,6)$ and $n = 5$.

Bivariate negative hupergeometric(N, D_1, D_2, D_3, r):

$$f_{X,Y}(x,y) = \frac{(r+x+y-1)!}{x!y!(r-1)!}\frac{(D_1)_x(D_2)_y(D_3)_r}{(N)_{x+y+r}}$$

where $D_1, D_2, D_3, N, r, x, y$ are integers, $D_1 + D_2 + D_3 = N$.

Bivariate Poisson(λ_1, λ_2):

$$f_{X,Y}(x,y) = \frac{\lambda_1^x \lambda_2^y}{x!y!}e^{-\lambda_1-\lambda_2}$$

where $0 < \lambda_1, \lambda_2 < \infty$, $x, y = 0, 1, \ldots, \infty$.

For a continuous example let

$$f_{X,Y}(x,y) = \frac{e^{-(x^2+y^2)/2}}{2\pi} \text{ for } -\infty < x, y < \infty\ .$$

Figure 7.2 plots this continuous joint density. This is called the bivariate normal $\mathcal{N}_2(\mathbf{0}, \mathbf{I_2})$ density where $\mathbf{0} = (0,0)$, and $\mathbf{I_2} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

Some important bivariate densities are:

Bivariate normal $\mathcal{N}_2(\mu, \mathbf{\Sigma})$ where $\mu = (\mu_1, \mu_2)$, $\mathbf{\Sigma} = \begin{pmatrix} \sigma^2 & \rho\sigma\tau \\ \rho\sigma\tau & \tau^2 \end{pmatrix}$

$$f_{X,Y}(x,y) = \frac{1}{2\pi\sigma\tau\sqrt{1-\rho^2}}e^{-\frac{1}{2(1-\rho^2)}\{\left(\frac{x-\mu_1}{\sigma}\right)^2 - 2\rho\left(\frac{x-\mu_1}{\sigma}\right)\left(\frac{y-\mu_2}{\tau}\right) + \left(\frac{y-\mu_2}{\tau}\right)^2\}}$$

and $-\infty < \mu_1, \mu_2 < \infty$, $0 < \sigma, \tau$, $-1 < \rho < 1$, $-\infty < x, y < \infty$.

Bivariate beta or Dirichlet$(\alpha_1, \alpha_2, \alpha_3)$:

$$f_{X,Y}(x,y) = \frac{\Gamma(\alpha_1+\alpha_2+\alpha_3)}{\Gamma(\alpha_1)\Gamma(\alpha_2)\Gamma(\alpha_3)}x^{\alpha_1-1}y^{\alpha_2-1}(1-x-y)^{\alpha_3-1}$$

for $\alpha_1, \alpha_2, \alpha_3 > 0$, $0 < x, y < 1$, $x + y < 1$.

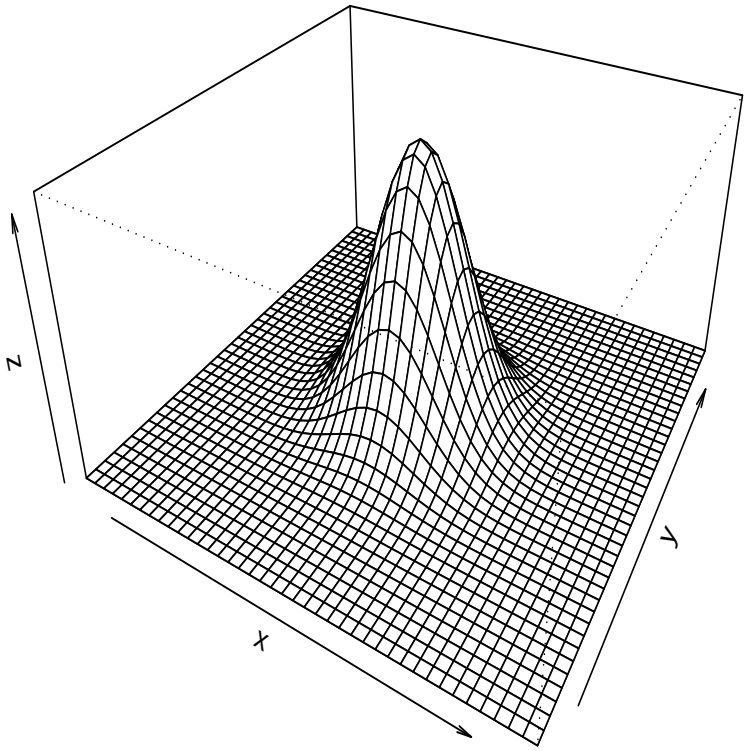

Figure 7.2: Bivariate Normal $\mathcal{N}_2(0, \mathbf{I}_2)$ Density.

7.1.1 Marginal Densities

The marginal density for a single discrete random variable can be obtained from the joint discrete density by summing

$$f_X(x) = \sum_{all\ y} p_{X,Y}(x,y), \quad f_Y(y) = \sum_{all\ x} f_{X,Y}(x,y)\ .$$

The marginal density for a continuous random variable is similarly obtained from the joint continuous density by integrating

$$f_X(x) = \int_{-\infty}^{\infty} f_{X,Y}(x,y)dy, \quad f_Y(y) = \int_{-\infty}^{\infty} f_{X,Y}(x,y)dx\ .$$

As examples, for the bivariate hypergeometric(N, D_1, D_2, D_3, n) the marginal is

$$f_X(x) = \sum_{y=L(x)}^{U(x)} \frac{\begin{pmatrix} D_1 \\ x \end{pmatrix}\begin{pmatrix} D_2 \\ y \end{pmatrix}\begin{pmatrix} D_3 \\ n-x-y \end{pmatrix}}{\begin{pmatrix} N \\ n \end{pmatrix}} = \frac{\begin{pmatrix} D_1 \\ x \end{pmatrix}\begin{pmatrix} D_2+D_3 \\ n-x \end{pmatrix}}{\begin{pmatrix} N \\ n \end{pmatrix}}$$

where $L(x) = \max\{0, n-x-D_3\}$ and $U(x) = \min\{D_2, n-x\}$.
This is a univariate hypergeometric(N, D_1, n) discrete density.

For the trinomial(m, p_1, p_2, p_3) the marginal is

$$f_X(x) = \begin{pmatrix} m \\ x \end{pmatrix} p_1^x (1-p_1)^{m-x}$$

which is the univariate binomial(m, p_1).

The bivariate negative binomial(r, p_1, p_2, p_3) has marginal

$$f_X(x) = \begin{pmatrix} x+r-1 \\ x \end{pmatrix}\left(\frac{p_1}{p_1+p_3}\right)^x\left(\frac{p_3}{p_1+p_3}\right)^r$$

which is the univariate negative binomial$(r, p_1/(p_1+p_3))$.

The bivariate negative hypergeometric(N, D_1, D_2, D_3, r) has

$$f_X(x) = \begin{pmatrix} x+r-1 \\ x \end{pmatrix}\frac{(D_1)_x(D_3)_r}{(D_1+D_3)_{x+r}}$$

which is the univariate negative hypergeometric(D_1+D_3, D_1, r).

The marginal of the bivariate normal $\mathcal{N}_2(\mathbf{0}, \mathbf{I_2})$ density is

$$f_X(x) = \int_{-\infty}^{\infty} \frac{1}{2\pi} e^{-(x^2+y^2)/2} dy = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$$

which is the univariate normal $\mathcal{N}(0, 1)$ density.

The marginal of the bivariate Dirichlet$(\alpha_1, \alpha_2, \alpha_3)$ is

$$f_X(x) = \frac{\Gamma(\alpha_1 + \alpha_2 + \alpha_3)}{\Gamma(\alpha_1)\Gamma(\alpha_2 + \alpha_3)} x^{\alpha_1 - 1}(1 - x)^{\alpha_2 + \alpha_3 - 1}$$

for $0 < x < 1$ which is the univariate beta$(\alpha_1, \alpha_2 + \alpha_3)$ density.

7.1.2 Conditional Densities

The conditional distribution of a random variable given the value of another random variable is defined for discrete random variables by

$$f_{X|Y}(x|y) = P(X = x|Y = y) = \frac{P(X = x,\ Y = y)}{P(Y = y)} = \frac{f_{X,Y}(x, y)}{f_Y(y)} \ .$$

For example, for the negative binomial with $p_3 = 1 - p_1 - p_2$, using the fact that negative binomial probabilities add to 1,

$$f_Y(y) = \sum_{x=0}^{\infty} \frac{(r + x + y - 1)!}{x!y!(r - 1)!} p_1^x p_2^y p_3^r$$

$$= \frac{(y + r - 1)!}{y!(r - 1)!} \left(\frac{p_2}{(1 - p_1)}\right)^y \left(\frac{p_3}{(1 - p_1)}\right)^r \sum_{x=0}^{\infty} \frac{(x + y + r - 1)!}{x!(y + r - 1)!} p_1^x (1 - p_1)^{y+r}$$

$$= \frac{(y + r - 1)!}{y!(r - 1)!} \left(\frac{p_2}{(1 - p_1)}\right)^y \left(\frac{p_3}{(1 - p_1)}\right)^r \ .$$

Then $f_{X|Y}(x|y) =$

$$\left(\frac{(r + x + y - 1)!}{x!y!(r - 1)!} p_1^x p_2^y p_3^r\right) / \left(\frac{(y + r - 1)!}{y!(r - 1)!} \left(\frac{p_2}{(1 - p_1)}\right)^y \left(\frac{p_3}{(1 - p_1)}\right)^r\right)$$

$$= \frac{(x + y + r - 1)!}{x!(y + r - 1)!} p_1^x (1 - p_1)^{y+r}$$

which is the negative binomial$(p_1, y + r)$.

For continuous random variables, the conditional density of X given Y is defined by

$$f_{X|Y}(x|y) = \frac{f_{X,Y}(x,y)}{f_Y(y)} \ .$$

For example, for the bivariate normal $\mathcal{N}_2(\mu, \mathbf{\Sigma})$, the marginal density

$$f_Y(y) = \int_{-\infty}^{\infty} \frac{1}{2\pi\sigma\tau\sqrt{1-\rho^2}} e^{-\frac{1}{2(1-\rho^2)}\{\left(\frac{x-\mu_1}{\sigma}\right)^2 - 2\rho\left(\frac{x-\mu_1}{\sigma}\right)\left(\frac{y-\mu_2}{\tau}\right) + \left(\frac{y-\mu_2}{\tau}\right)^2\}} dx$$

and setting $u = (x-\mu_1)/(\sigma\sqrt{1-\rho^2})$

$$= \frac{e^{-(y-\mu_2)^2/(2\tau^2)}}{\tau\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-\frac{1}{2}\{u-\rho(y-\mu_2)/(\tau\sqrt{1-\rho^2})\}^2} du = \frac{e^{-(y-\mu_2)^2/(2\tau^2)}}{\tau\sqrt{2\pi}}$$

which is the univariate normal $\mathcal{N}(\mu_2, \tau^2)$ density. Then $f_{X|Y}(x|y) =$

$$\left(\frac{1}{2\pi\sigma\tau\sqrt{1-\rho^2}} e^{-\frac{1}{2(1-\rho^2)}\{\left(\frac{x-\mu_1}{\sigma}\right)^2 - 2\rho\left(\frac{x-\mu_1}{\sigma}\right)\left(\frac{y-\mu_2}{\tau}\right) + \left(\frac{y-\mu_2}{\tau}\right)^2\}}\right) \Big/ \left(\frac{1}{\tau\sqrt{2\pi}} e^{-\frac{(y-\mu_2)^2}{2\tau^2}}\right)$$

$$= \frac{1}{\sigma\sqrt{1-\rho^2}\sqrt{2\pi}} e^{-\frac{1}{2\sigma^2(1-\rho^2)}\{x-(\mu_1+\rho\sigma(y-\mu_2)/\tau)\}^2}$$

the univariate normal $\mathcal{N}(\mu_1 + \rho\sigma(y-\mu_2)/\tau, \sigma^2(1-\rho^2))$ conditional density.

We say the random variables X, Y are **independent** if

$$P(X \in B_1,\ Y \in B_2) = P(X \in B_1)P(Y \in B_2) \ .$$

For discrete or continuous random variables, X, Y are independent if the discrete or continuous densities factor:

$$f_{X,Y}(x,y) = f_X(x)f_Y(y) \text{ for all } (x,y) \ .$$

Equivalently, if the conditional density of $X|Y$ is the same as the marginal density of X, then X, Y are independent.

For example the bivariate Poisson satisfies the condition for independence since

$$f_{X,Y}(x,y) = \frac{\lambda_1^x \lambda_2^y}{x!y!} e^{-\lambda_1-\lambda_2} = \frac{\lambda_1^x}{x!} e^{-\lambda_1} \times \frac{\lambda_2^y}{y!} e^{-\lambda_2} = f_X(x)f_Y(y) \ .$$

When $\rho = 0$ the bivariate normal $\mathcal{N}_2(\mu, \mathbf{\Sigma})$ factors since $f_{X,Y}(x, y) =$

$$\frac{1}{2\pi\sigma\tau} e^{-\frac{1}{2}\{(x-\mu_1)^2/\sigma^2+(y-\mu_2)^2/\tau^2\}} = \left(\frac{e^{-\frac{1}{2\sigma^2}(x-\mu_1)^2}}{\sigma\sqrt{2\pi}}\right)\left(\frac{e^{-\frac{1}{2\tau^2}(y-\mu_2)^2}}{\tau\sqrt{2\pi}}\right) = f_X(x)f_Y(y)$$

and we have independence. The parameter ρ is called the correlation coefficient and is a measure of dependence.

7.2 Several Random Variables

For several random variables $X_1, X_2, \ldots, X_n$ the joint discrete or continuous density is an n dimensional function

$$f_{X_1,X_2,\ldots,X_n}(x_1, x_2, \ldots, x_n)$$

that is non negative and sums or integrates to 1 over the n dimensional set of points $(x_1, x_2, \ldots, x_n)$. There are $2^n - 2$ subsets of $2, 3, \ldots, n-1$ variables and that many possible marginal densities. For example if $n = 3$ there are univariate marginals for X_1, for X_2, and for X_3 and bivariate marginals for (X_1, X_2), for (X_1, X_3), and for (X_2, X_3).

7.2.1 Discrete Multivariate Distributions

Some discrete multivariate examples are

Multinomial$(m, p_1, p_2, \ldots, p_k)$

$$f_{X_1,X_2,\ldots,X_{k-1}}(x_1, x_2, \ldots, x_{k-1}) = \frac{m!}{\prod_{j=1}^k x_j!} \prod_{j=1}^k p_j^{x_j}$$

for $0 < p_i < 1$, $p_1 + p_2 + \cdots + p_k = 1$, and integer x_i satisfy $0 \le x_i \le m$, $x_1 + x_2 + \cdots + x_{k-1} \le m$, and $x_k = m - \sum_{j=1}^{k-1} x_j$.

Multivariate hypergeometric$(N, D_1, D_2, \ldots, D_k, m)$

$$f_{X_1,X_2,\ldots,X_{k-1}}(x_1, x_2, \ldots, x_{k-1}) = \frac{m!(D_1)_{x_1}(D_2)_{x_2}\cdots(D_{k-1})_{x_{k-1}}(D_k)_{x_k}}{x_1!x_2!\cdots x_k!(N)_m}$$

for $D_1 + D_2 + \cdots + D_k = N$ and integer x_i satisfy $0 \le x_i \le m$, $x_1 + x_2 + \cdots + x_k = m$.

Multivariate negative binomial$(r, p_1, p_2, \ldots p_k)$

$$f_{X_1,X_2,\ldots,X_{k-1}}(x_1, x_2, \ldots, x_{k-1}) = \frac{(x_1 + x_2 + \cdots + x_{k-1} + r - 1)!}{x_1!x_2! \cdots x_{k-1}!(r-1)!} p_1^{x_1} p_2^{x_2} \cdots p_{k-1}^{x_{k-1}} p_k^r$$

for $0 < p_i < 1$, $p_1 + p_2 + \cdots + p_k = 1$, and integer x_i satisfy $0 \leq x_i < \infty$.

Multivariate negative hypergeometic$(N, D_1, D_2, \ldots, D_k, r)$

$$f_{X_1,X_2,\ldots,X_{k-1}}(x_1, x_2, \ldots, x_{k-1}) =$$
$$\frac{(x_1 + x_2 + \cdots + x_{k-1} + r - 1)!}{x_1!x_2! \cdots x_{k-1}!(r-1)!} \frac{(D_1)_{x_1}(D_2)_{x_2} \cdots (D_{k-1})_{x_{k-1}}(D_k)_r}{(N)_{(m+x_1+x_2+\cdots+x_{k-1})}}$$

for integer $D_i > 0$, $D_1 + D_2 + \cdots + D_k = N$, and integer x_i satisfy $0 \leq x_i < \infty$.

7.2.2 Continuous Multivariate Distributions

Some continuous multivariate examples are

Multivariate normal $\mathcal{N}_n(\mu,\ \mathbf{\Sigma})$,

$$\mu = (\mu_1, \mu_2, \ldots, \mu_n)^T, \text{ and } \mathbf{\Sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \ldots & \sigma_{1n} \\ \sigma_{21} & \sigma_{22} & \ldots & \sigma_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{n1} & \sigma_{n2} & \ldots & \sigma_{nn} \end{pmatrix}$$

where $\mathbf{\Sigma}$ is symmetric and positive definite. The symmetric condition is $\sigma_{ij} = \sigma_{ji}$. In matrix notation $\mathbf{\Sigma} = \mathbf{\Sigma^T}$ where $\mathbf{\Sigma^T}$ is the transpose matrix obtained by interchanging rows and columns. The positive definite condition says that for all vectors $(v_1, v_2, \ldots, v_n)^T$ with some component $v_j \neq 0$, we have

$$\sum_{i=1}^{n} \sum_{j=1}^{n} v_i \sigma_{ij} v_j > 0 \ .$$

$$f_{X_1,X_2,\ldots,X_n}(x_1, x_2, \ldots, x_n) = \frac{1}{(2\pi)^{n/2}|\mathbf{\Sigma}|^{1/2}} \exp\{-\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} (x_i - \mu_i)\sigma^{(ij)}(x_j - \mu_j)\}$$

where $\mathbf{\Sigma^{-1}} = (\sigma^{(ij)} \ : i, j = 1, 2, \ldots, n)$ is the inverse matrix for $\mathbf{\Sigma}$ and $|\mathbf{\Sigma}|$ is the determinant of $\mathbf{\Sigma}$. The inverse matrix satisfies

$$\sum_{k=1}^{n} \sigma_{ik}\sigma^{(kj)} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \quad \text{or } \mathbf{\Sigma\Sigma^{-1}} = \mathbf{I_n}$$

where the identity matrix with n rows and n columns is

$$\mathbf{I_n} = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix} .$$

Multivariate Dirichlet$(\alpha_1, \alpha_2, \ldots, \alpha_n, \alpha_{n+1})$ where $\alpha_i > 0$

$$f_{X_1,X_2,\ldots,X_n}(x_1, x_2, \ldots, x_n) = \frac{\Gamma(\sum_{i=1}^{n+1} \alpha_i)}{\prod_{i=1}^{n+1} \Gamma(\alpha_i)} \left(\prod_{i=1}^{n} x_i^{\alpha_i - 1} \right) (1 - \sum_{i=1}^{n} x_i)^{\alpha_{n+1}-1}$$

for $0 < x_i < 1$, $\sum_{i=1}^{n} x_i < 1$.

Many other examples are obtained by assuming $X_1, X_2, \ldots, X_n$ are independent identically distributed with density f so that

$$f_{X_1,X_2,\ldots,X_n}(x_1, x_2, \ldots, x_n) = \prod_{i=1}^{n} f(x_i) .$$

7.3 Problems

1. Derive the marginal distribution of X for the bivariate negative binomial(r, p_1, p_2, p_3) distribution.

2. For the three dimensional multinomial(m, p_1, p_2, p_3, p_4) derive the marginal joint distribution for X_1, X_2.

3. For the bivariate Dirichlet$(\alpha_1, \alpha_2, \alpha_3)$ derive the marginal density for X.

4. For the bivariate Dirichlet, derive the conditional density for X given $Y = y$.

5. For the multivariate normal $\mathcal{N}_n(\mu, \mathbf{\Sigma})$ show that if $\mathbf{X} = (\mathbf{X_1^{1\times m}}, \mathbf{X_2^{1\times(n-m)}})$ that X_1 and X_2 are independent if

$$\mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma_{11}} & \mathbf{0} \\ \mathbf{0} & \mathbf{\Sigma_{22}} \end{pmatrix}$$

by showing $f_{\mathbf{X}}(\mathbf{x}) = f_{\mathbf{X_1}}(\mathbf{x_1}) f_{\mathbf{X_2}}(\mathbf{x_2})$.

Chapter 8

Characteristic Functions

8.1 Univariate Characteristic Functions

A very convenient technical device is the complex valued characteristic function

$$h_X(t) = E(e^{itX}) = E(\cos(tX)) + iE(\sin(tX))$$

where $i = \sqrt{-1}$. There is a 1-1 correspondence between a distribution and its characteristic function. It always exists since

$$|e^{itX}| = (\cos^2(tX) + \sin^2(tX))^{1/2} = 1 \ .$$

Theorem 8.1 *If $h_X(u)$ is the characteristic function of the distribution function $F_X(x)$, then*

$$F_X(b) - F_X(a) = \frac{1}{2\pi} \lim_{c\to\infty} \int_{-c}^{c} \frac{(e^{-iua} - e^{-iub})}{iu} h_X(u)du$$

for all a, b at which F_X is continuous.

Proof.
Define

$$I_c = \frac{1}{2\pi} \int_{-c}^{c} \frac{(e^{-iua} - e^{-iub})}{iu} \left[\int_{-\infty}^{\infty} e^{iux} dF_X(x) \right] du \ .$$

Since

$$\left| \frac{(e^{-iua} - e^{-iub})}{iu} e^{iux} \right| = \left| \frac{(e^{-iua} - e^{-iub})}{iu} \right| = \left| \int_a^b e^{-iux} dx \right| \leq b - a$$

and

$$\int_{-c}^{c}\int_{-\infty}^{\infty}(b-a)dF_X(x) = 2c(b-a) < \infty$$

we can interchange the order of integration (Fubini's theorem) to get

$$I_c = \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-c}^{c}\frac{(e^{-iua}-e^{-iub})}{iu}e^{iux}dudF_X(x) = \int_{-\infty}^{\infty}J_c(x)dF_X(x)$$

where

$$J_c(x) = \frac{1}{2\pi}\int_{-c}^{c}\frac{(\sin(u(x-a))-\sin(u(x-b)))}{u}du$$

since

$$\int_{-c}^{c}\frac{(\cos(u(x-a))-\cos(u(x-b)))}{iu}du = 0\ .$$

Substituting $v = u(x-a)$ and $w = u(x-b)$ we get

$$J_c(x) = \frac{1}{2\pi}\int_{-c(x-a)}^{c(x-a)}\frac{\sin(v)}{v}dv - \frac{1}{2\pi}\int_{-c(x-b)}^{c(x-b)}\frac{\sin(w)}{w}dw\ .$$

As $c \to \infty$ we have

$$J_c(x) \longrightarrow J(x) = \begin{cases} 0 & \text{if } x < a \text{ or } x > b \\ 1/2 & \text{if } x = a \text{ or } x = b \\ 1 & \text{if } a < x < b. \end{cases}$$

Using the dominated convergence, for a, b continuity points of F_X,

$$\lim_{c\to\infty} I_c = \int_{-\infty}^{\infty}J(x)dF_X(x) = F_X(b) - F_X(a)\ . \blacksquare$$

For integer valued discrete random variables the p.d.f. satisfies

$$f_X(x) = \frac{1}{2\pi}\int_{-\pi}^{\pi}h_X(t)e^{-itx}dt. \tag{8.1}$$

For continuous random variables we have

$$f_X(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}h_X(t)e^{-itx}dt \tag{8.2}$$

provided its characteristic function $h_X(t)$ satisfies$\int_{-\infty}^{\infty} |h_X(t)|dt < \infty$. As examples, the characteristic function for a binomial random variable is

$$h_X(t) = \sum_{x=0}^{n} e^{itx} \binom{n}{x} p^x q^{n-x} = (pe^{it} + q)^n$$

and equation (8.1) is verified

$$\binom{n}{x} p^x q^{n-x} = \frac{1}{2\pi} \int_{-\pi}^{\pi} \sum_{k=0}^{n} e^{itk} \binom{n}{k} p^k q^{n-k} e^{-itx} dt$$

since

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} e^{it(k-x)} dt = \begin{cases} 1 & \text{if } k = x \\ 0 & \text{if } k \neq x \end{cases}$$

The characteristic function for the density $f_X(x) = e^{-x^2/2}/\sqrt{2\pi}$ is $h_X(t) = e^{-t^2/2}$. To verify equation (8.2) in this case

$$f_X(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-t^2/2} e^{-itx} dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-t^2/2} \cos(tx) dt$$

since the imaginary part

$$-i \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-t^2/2} \sin(tx) dt = 0$$

is the integral of an odd function with the integral on the negative axis canceling the integral on the positive axis.
If we differentiate with respect to x we get

$$f'_X(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-t^2/2} (-t \sin(tx)) dt$$

and integrating by parts

$$= \frac{1}{2\pi} e^{-t^2/2} \sin(tx)|_{-\infty}^{\infty} - \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-t^2/2} x \cos(tx) dt = -x f_X(x) \ .$$

Solving the differential equation

$$f'_X(x) = -x f_X(x) \text{ where } f_X(0) = \frac{1}{\sqrt{2\pi}}$$

we get after integrating, $\log_e(f_X(x)) = -x^2/2 + C$ where $C = \log_e(1/\sqrt{2\pi})$. Thus $f_X(x) = e^{-x^2/2}/\sqrt{2\pi}$.

Theorem 8.2 *If $E(|X^n|) = \mu_n < \infty$ then for $k \leq n$*

$$h_X^{(k)}(u) = i^k \int e^{iux} x^k dF(x), \quad u \in R$$

and $h_X^{(k)}$ is continuous and bounded by $\mu_k < \infty$. Also

$$h_X(u) = \sum_{k=0}^{n-1} m_k \frac{(iu)^k}{k!} + u^n \int_0^1 \frac{(1-t)^{n-1}}{(n-1)!} h_X^{(n)}(tu) dt = \sum_{k=0}^{n} m_k \frac{(iu)^k}{k!} + o(u^n)$$

where $m_n = E(X^n)$.

Proof.
First, since $|X|^k \leq 1 + |X|^n$ for $k \leq n$, $\mu_n < \infty$ gives $\mu_k < \infty$. If we differentiate $\int e^{iux} dF(x)$ a total of k times, the integral is absolutely convergent and by the dominated convergence theorem, we can interchange the differentiation limit and the integration:

$$h_X^{(k)}(u) = \frac{d}{du} h_X^{(k-1)}(u) = \lim_{\delta \downarrow 0} \frac{h_X^{(k-1)}(u+\delta) - h_X^{(k-1)}(u)}{\delta}$$

$$= \int (ix)^{k-1} \lim_{\delta \downarrow 0} \frac{(e^{ix(u+\delta)} - e^{ixu})}{\delta} dF(x) = i^k \int e^{iux} x^k dF(x) \ .$$

If we expand

$$e^{iux} = \sum_{k=0}^{n-1} \frac{(iux)^k}{k!} + u^n \int_0^1 \frac{(1-t)^{n-1}}{(n-1)!} (ix)^n e^{iutx} dt$$

and integrate, we get

$$h_X(u) = \sum_{k=0}^{n-1} \frac{(iu)^k}{k!} m_k + u^n \int_0^1 \frac{(1-t)^{n-1}}{(n-1)!} h_X^{(n)}(tu) dt \ .$$

Similarly, if we expand

$$e^{iux} = \sum_{k=0}^{n} \frac{(iux)^k}{k!} + \frac{(iu)^{n+1}}{(n+1)!} e^{iu\xi} \text{ where } 0 \leq \xi \leq x$$

then after integration, we get

$$h_X(u) = \sum_{k=0}^{n} \frac{(iu)^k}{k!} m_k + o(u^n) \ . \blacksquare$$

As an example, for the binomial(n, p)

$$h'_X(0) = \frac{d}{dt}(pe^{it} + q)^n|_{t=0} = n(pe^{it} + q)^{n-1} ipe^{it}|_{t=0} = inp$$

so $E(X) = np$.
For the standard normal $\mathcal{N}(0, 1)$

$$h''_X(0) = \frac{d^2}{dt^2} e^{-t^2/2}|_{t=0} = (t^2 - 1)e^{-t^2/2}|_{t=0} = -1 = i^2 1$$

so $E(X^2) = 1$.

The following is a list of some useful characteristic functions:

Binomial(n, p): $h_X(t) = (pe^{it} + q)^n$.

Negative binomial(r, p): $h_Y(t) = (p/(1 - qe^{it}))^r$.

Poisson(λ): $h_X(t) = \exp\{\lambda(e^{it} - 1)\}$

Normal $\mathcal{N}(\mu, \sigma^2)$: $h_X(t) = \exp\{it\mu - t^2\sigma^2/2\}$.

Gamma(α, σ): $h_X(t) = (1 - it\sigma)^{-\alpha}$.

Cauchy(μ, σ): $h_X(t) = \exp\{it\mu - \sigma|t|\}$.

We note for the Cauchy, the derivative of $h_X(t)$ does not exist at $t = 0$ and $E(X)$ does not exist since $E(|X|) = \infty$.

The moment generating function, when it exists. is defined by

$$m_X(t) = E(e^{tX}) \ .$$

Theorem 8.3 *If the moment generating function exists and is finite in an open interval $(-a, a)$ about $t = 0$, then the characteristic function is*

$$h_X(t) = m_X(it).$$

Proof.
If $z = u + iv$ is a complex variable with $u \in (-a, a)$ and we substitute into m_X to get the complex function

$$m_X(z) = \int_{-\infty}^{\infty} e^{zx} dF_X(x)$$

then we first show $m_X(z)$ is an analytic function of z.
We have

$$|m_X(z)| \leq \int_{-\infty}^{\infty} |e^{zx}| dF_X(x) = \int_{-\infty}^{\infty} e^{ux} dF_X(x) = m_X(u) < \infty \ .$$

Next

$$\frac{(m_X(z+\delta) - m_X(z))}{\delta} = \int_{-\infty}^{\infty} e^{zx} \frac{(e^{\delta x} - 1)}{\delta} dF_X(x) \ .$$

Using the inequality (which can be proved by a series argument)

$$\left| \frac{(e^{\delta x} - 1)}{\delta} \right| \leq \frac{e^{\eta |x|}}{\eta}, \text{ for } |\delta| \leq \eta$$

we have the integrand bounded in absolute value by

$$\left| e^{zx} \frac{(e^{\delta x} - 1)}{\delta} \right| \leq \frac{1}{\eta} \left| \exp\{zx + \eta |x|\} \right| \leq \frac{1}{\eta} \left| \exp\{(z+\eta)x\} + \exp\{(z-\eta)x\} \right|$$

for $|\delta| \leq \eta$. For $\eta > 0$ sufficiently small, this is an integrable function and the dominated convergence theorem gives

$$\lim_{|\delta| \to 0} \frac{(m_X(z+\delta) - m_X(z))}{\delta} = \int_{-\infty}^{\infty} x e^{zx} dF_X(x)$$

finite and $m_X(z)$ is analytic.
Next, by the assumption, since $m_X(u) < \infty$ for real $u \in (-a, a)$ where $a > 0$, we have $m_X(z)$ is analytic for complex $z = u + iv$ where
$-a < u < a$, $-\infty < v < \infty$. By analytic continuation, $m_X(u)$ can be uniquely extended to the purely complex characteristic function

$$m_X(iv) = \int_{-\infty}^{\infty} e^{ivx} dF_X(x) = h_X(v), \text{ for } -\infty < v < \infty \ . \blacksquare$$

As an example, for the gamma distribution, the moment generating function is

$$m_X(t) = \int_0^\infty e^{tx} \frac{x^{\alpha-1} e^{-x/\sigma}}{\sigma^\alpha \Gamma(\alpha)} dx = (1 - t\sigma)^{-\alpha}$$

which is obtained by a change of variable. Replacing t by it gives $h_X(t) = (1 - it\sigma)^{-\alpha}$.

Another method to derive characteristic functions uses the Cauchy residue theorem for complex variables

$$2\pi i f(z_0) = \int_{z \in \mathcal{C}} \frac{f(z)}{(z - z_0)} dz$$

for a closed counter clockwise path $\mathcal{C}$ around the fixed point z_0.

To illustrate for the Cauchy$(0, 1)$ density, for $t > 0$,

$$e^{-t} = 2\pi i \left(\frac{e^{iti}}{\pi(i + i)} \right) = \int_{z \in \mathcal{C}} \frac{e^{itz}/(\pi(z + i))}{(z - i)} dz$$

$$= \int_{-R}^{R} \frac{e^{itx}}{\pi(1 + x^2)} dx + \int_0^\pi \frac{e^{it(Re^{i\theta})}}{\pi(1 + (Re^{i\theta})^2)} Re^{i\theta} i d\theta$$

$$\longrightarrow \int_{-\infty}^{\infty} \frac{e^{itx}}{\pi(1 + x^2)} dx = h_X(t) \text{ as } R \to \infty$$

since

$$\left| \int_0^\pi \frac{e^{it(Re^{i\theta})}}{\pi(1 + (Re^{i\theta})^2)} Re^{i\theta} i d\theta \right| \leq \frac{\pi R}{|R^2 - 1|} \to 0 \text{ as } R \to \infty \ .$$

The path $\mathcal{C}$ is illustrated in figure 8.1.

A similar argument with a path around $z = -i$ can be used to get $h_X(t) = e^t$ for $t < 0$. Combining, gives $h_X(t) = e^{-|t|}$ for $-\infty < t < \infty$ since $h_X(0) = 1$. We note that the moment generating function does not exist for the Cauchy so that we cannot use $h_X(t) = m_X(it)$.

In general, for $Y = aX + b$ we have $h_Y(t) = e^{itb} h_X(at)$. Thus for the Cauchy(μ, σ) the characteristic function is $e^{it\mu} e^{-|\sigma t|}$.

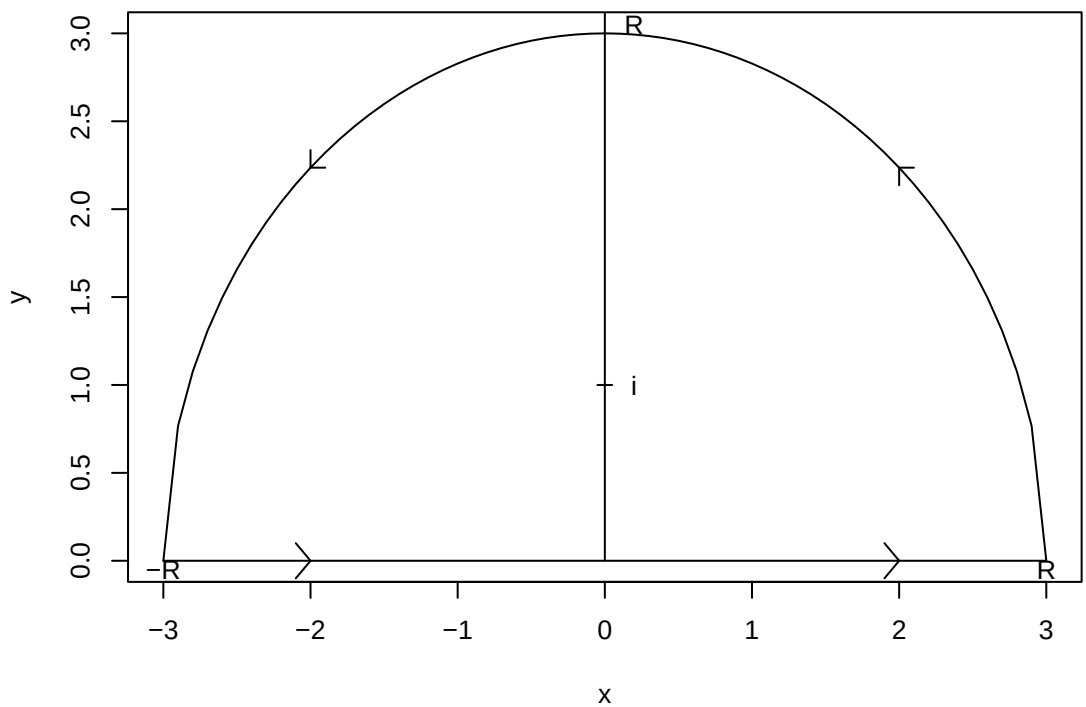

Figure 8.1: Counter clockwise path $\mathcal{C}$ used to calculate the Cauchy$(0,1)$ characteristic function $h_X(t)$ for $t > 0$.

8.2 Multivariate Characteristic Functions

The multivariate characteristic function is defined by

$$h_{X_1,X_2,\ldots,X_n}(t_1,t_2,\ldots,t_n) = E(e^{i(t_1X_1+t_2X_2+\cdots+t_nX_n)}) \ .$$

The inversion formula for discrete random vectors with integer valued components is

$$f_{X_1,X_2,\ldots,X_n}(x_1,x_2,\ldots,x_n) =$$

$$\left(\frac{1}{2\pi}\right)^n \int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\cdots\int_{-\pi}^{\pi} e^{-i(t_1x_1+t_2x_2+\cdots+t_nx_n)} h_{X_1,x_2,\ldots,X_n}(t_1,t_2,\ldots,t_n)dt_1dt_2\cdots dt_n \ .$$

For continuous random variables

$$f_{X_1,X_2,\ldots,X_n}(x_1,x_2,\ldots,x_n) =$$

$$\left(\frac{1}{2\pi}\right)^n \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-i(t_1x_1+t_2x_2+\cdots+t_nx_n)} h_{X_1,X_2,\ldots,X_n}(t_1,t_2,\ldots,t_n)dt_1dt_2\cdots dt_n$$

provided

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} |h_{X_1,X_2,\ldots,X_n}(t_1,t_2,\ldots,t_n)|dt_1dt_2\cdots dt_n < \infty \ .$$

The general multivariate inversion formula is

Theorem 8.4 *If* $\mathbf{a} = (a_1, a_2, \ldots a_n)$ *and* $\mathbf{b} = (b_1, b_2, \ldots, b_n)$, $a_i < b_i$, *are continuity points of* $F_{X_1,X_2,\ldots,X_n}(x_1,x_2,\ldots,x_n)$ *then for* $\mathbf{X} = (X_1, X_2, \ldots, X_n)$, $\mathbf{u} = (u_1, u_2, \ldots, u_n)$

$$F_{\mathbf{X}}(\mathbf{b}) - F_{\mathbf{X}}(\mathbf{a}) = \lim_{c\to\infty} \frac{1}{(2\pi)^n}\int_{-c}^{c}\cdots\int_{-c}^{c}\left[\prod_{k=1}^{n}\frac{(e^{-iu_ka_k} - e^{-iu_kb_k})}{iu_k}\right] h_{\mathbf{X}}(\mathbf{u})d\mathbf{u} \ .$$

Proof.
Following the proof and notation of the univariate inversion theorem 8.1,

$$\frac{1}{(2\pi)^n}\int_{-c}^{c}\cdots\int_{-c}^{c}\left[\prod_{k=1}^{n}\frac{(e^{-iu_ka_k} - e^{-iu_kb_k})}{iu_k}\right] h_{\mathbf{X}}(\mathbf{u})d\mathbf{u} = \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\left[\prod_{k=1}^{n} J_c(x_k)\right] dF_{\mathbf{X}}(\mathbf{x})$$

$$\longrightarrow \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\left[\prod_{k=1}^{n} J(x_k)\right] dF_{\mathbf{X}}(\mathbf{x}) = F_{\mathbf{X}}(\mathbf{b}) - F_{\mathbf{X}}(\mathbf{a}) \ . \blacksquare$$

The multivariate moment generating function is

$$m_{\mathbf{X}}(u_1,u_2,\ldots,u_n) = E(e^{\sum_{k=1}^{n} u_kX_k}) \ .$$

An extension of theorem 8.3 to the multivariate case is

Theorem 8.5 *If the multivariate moment generating* $m_{\mathbf{X}}(\mathbf{u})$ *exists for* $\mathbf{u} = (u_1, u_2, \ldots, u_n)$ *in a neighborhood of* $\mathbf{u} = (0, 0, \ldots, 0)$ *then the multivariate characteristic function can be obtained by replacing* u_k *by* iu_k *in the moment generating function:*

$$h_{\mathbf{X}}(u_1,u_2,\ldots,u_n) = m_{\mathbf{X}}(iu_1,iu_2,\ldots,iu_n) \ .$$

Proof.
Consider the univariate moment generating function for a linear combination

$$E(e^{t\sum_{k=1}^{n} a_k X_k}) = m_{X_1,X_2,\ldots,X_n}(ta_1, ta_2, \ldots, ta_n) \ .$$

By the univariate theorem 8.3, the corresponding characteristic function is

$$E(e^{it\sum_{k=1}^{n} a_k X_k}) = m_{X_1,X_2,\ldots,X_n}(ita_1, ita_2, \ldots, ita_n) \ .$$

But this is just the characteristic function

$$h_{X_1,X_2,\ldots,X_n}(ta_1, ta_2, \ldots ta_n) \ . \blacksquare$$

For examples of characteristic functions, for the multinomial $(m, p_1, p_2, \ldots, p_k)$ with $x_k = m - \sum_{j=1}^{k-1} x_j$ it is $h_{X_1,X_2,\ldots,X_{k-1}}(t_1, t_2, \ldots, t_{k-1}) =$

$$\sum_{x_{k-1}} \sum_{x_{k-2}} \cdots \sum_{x_1} e^{i\sum_{j=1}^{k-1} t_j x_j} \frac{m!}{\prod_{j=1}^{k} x_j!} \prod_{j=1}^{k} p_j^{x_j} = \left(p_k + \sum_{j=1}^{k-1} p_j e^{it_j} \right)^m \ .$$

The multivariate negative binomial $(r, p_1, p_2, \ldots p_k)$ characteristic function is

$$h_{X_1,X_2,\ldots,X_{k-1}}(t_1, t_2, \ldots, t_{k-1}) = \left(\frac{p_k}{1 - \sum_{j=1}^{k-1} e^{it_j} p_j} \right)^r \ .$$

The characteristic function for the multivariate normal $\mathcal{N}_n(\mu, \mathbf{\Sigma})$ is

$$h_{X_1,X_2,\ldots,X_n}(t_1, t_2, \ldots, t_n) = \exp\{i \sum_{j=1}^{n} \mu_j t_j - \frac{1}{2} \sum_{j=1}^{n} \sum_{k=1}^{n} t_j \sigma_{jk} t_k\}$$

$$= \exp\{i \mathbf{t^T} \mu - \frac{1}{2} \mathbf{t^T \Sigma t}\}$$

where $\mathbf{t}^T = (t_1, t_2, \ldots, t_n)$.

The multivariate characteristic function can be used to obtain the marginal distribution for a subset of variables using

$$h_{X_1,X_2,\ldots,X_m}(t_1, t_2, \ldots, t_m) = h_{X_1,X_2,\ldots,X_m,X_{m+1},\ldots,X_n}(t_1, t_2, \ldots, t_m, 0, \ldots, 0)$$

for $m < n$.

For example, the marginals of the multivariate normal are also multivariate normal. If $X_1, X_2, \ldots, X_n$ are $\mathcal{N}_n(\mu, \mathbf{\Sigma})$ we can partition $(\mathbf{t}^{n\times 1})^T = ((\mathbf{t}_1^{m\times 1})^T, (\mathbf{t}_2^{(n-m)\times 1})^T)$

$$\boldsymbol{\mu} = \begin{pmatrix} \boldsymbol{\mu}_1^{m\times 1} \\ \boldsymbol{\mu}_2^{(n-m)\times 1} \end{pmatrix}, \quad \text{and } \mathbf{\Sigma}^{\mathbf{n}\times\mathbf{n}} = \begin{pmatrix} \mathbf{\Sigma}_{\mathbf{11}}^{\mathbf{m}\times\mathbf{m}} & \mathbf{\Sigma}_{\mathbf{12}}^{\mathbf{m}\times(\mathbf{n}-\mathbf{m})} \\ \mathbf{\Sigma}_{\mathbf{21}}^{(\mathbf{n}-\mathbf{m})\times\mathbf{m}} & \mathbf{\Sigma}_{\mathbf{22}}^{(\mathbf{n}-\mathbf{m})\times(\mathbf{n}-\mathbf{m})} \end{pmatrix}$$

and get

$$h_{X_1,X_2,\ldots,X_m}(\mathbf{t}_1^{m\times 1}) = h_{X_1,X_2,\ldots X_n}(\mathbf{t}_1^T, \mathbf{0}) = \exp\{i\mathbf{t}_1^T\boldsymbol{\mu}_\mathbf{1} - \frac{1}{2}\mathbf{t}_1^T\mathbf{\Sigma}_{11}^{m\times m}\mathbf{t}_1\} \ .$$

The marginal is thus the multivariate normal $\mathcal{N}_m(\boldsymbol{\mu}_1, \mathbf{\Sigma}_{11})$.

8.2.1 Conditional Characteristic Functions

In the bivariate case, the conditional characteristic function is

$$h_{X|Y}(t|y) = \sum_{all\ x} e^{itx} p_{X|Y}(x|y) \text{ and } h_{X|Y}(t|y) = \int_{-\infty}^{\infty} e^{itx} f_{X|Y}(x|y)dx \quad (8.3)$$

for discrete and continuous distributions respectively. We can obtain them from the joint characteristic function by

$$h_{X|Y}(t|y) = \frac{\int_{-\pi}^{\pi} e^{-iys} h_{X,Y}(t,s)ds}{\int_{-\pi}^{\pi} e^{-iys} h_{X,Y}(0,s)ds} \quad (8.4)$$

for discrete random vectors with integer components and

$$h_{X|Y}(t|y) = \frac{\int_{-\infty}^{\infty} e^{-iys} h_{X,Y}(t,s)ds}{\int_{-\infty}^{\infty} e^{-iys} h_{X,Y}(0,s)ds}$$

for the continuous case.

For the multivariate case, writing $\mathbf{X}^{\mathbf{1}\times\mathbf{n}} = (\mathbf{X}_\mathbf{1}^{\mathbf{1}\times\mathbf{m}}, \mathbf{X}_\mathbf{2}^{\mathbf{1}\times(\mathbf{n}-\mathbf{m})})$, $\mathbf{t}^{\mathbf{1}\times\mathbf{n}} = (\mathbf{t}_\mathbf{1}^{\mathbf{1}\times\mathbf{m}}, \mathbf{t}_\mathbf{2}^{\mathbf{1}\times(\mathbf{n}-\mathbf{m})})$

$$h_{\mathbf{X_1}|\mathbf{X_2}}(\mathbf{t_1}|\mathbf{x_2}) =$$

$$\frac{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-i(\mathbf{t_2}\mathbf{x_2^T})} h_{\mathbf{X_1},\mathbf{X_2}}(\mathbf{t_1},\mathbf{t_2})dt_{m+1}dt_{m+2}\cdots dt_n}{\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} e^{-i(\mathbf{t_2}\mathbf{x_2^T})} h_{\mathbf{X_1},\mathbf{X_2}}(\mathbf{0},\mathbf{t_2})dt_{m+1}dt_{m+2}\cdots dt_n}$$

for the continuous case with a similar formula for the discrete integer valued vector case with integration limits from $-\pi$ to π instead of $-\infty$ to ∞.

For an example, consider the bivariate trinomial(m, p_1, p_2, p_3) distribution and its conditional characteristic function given $Y = y$. Using formula (8.4) for random vectors with integer component values

$$h_{X|Y}(t|y) = \frac{\int_{-\pi}^{\pi} e^{-isy}(p_1 e^{it} + p_2 e^{is} + p_3)^m ds}{\int_{-\pi}^{\pi} e^{-isy}(p_1 + p_2 e^{is} + p_3)^m ds}$$

$$= \frac{\int_{-\pi}^{\pi} e^{-isy} \sum_j \sum_k \frac{m!}{j!k!(m-j-k)!}(p_1 e^{it})^j (p_2 e^{is})^k p_3^{(m-j-k)}}{\int_{-\pi}^{\pi} e^{-isy} \sum_j \frac{m!}{j!(m-j)!}(p_2 e^{is})^j (p_1 + p_3)^{(m-j)} ds}$$

$$= \frac{\frac{1}{2\pi} \sum_j \frac{m!}{j!y!(m-y-j)!}(p_1 e^{it})^j (p_2 e^{is})^y p_3^{(m-y-j)}}{\frac{1}{2\pi} \frac{m!}{y!(m-y)!}(p_2 e^{is})^y (p_1 + p_3)^{(m-y)}}$$

$$= \frac{\sum_j \frac{(m-y)!}{j!(m-y-j)!}(p_1 e^{it})^j p_3^{(m-y-j)}}{(p_1 + p_3)^{(m-y)}} = \left(\frac{p_1}{p_1 + p_3} e^{it} + \frac{p_3}{p_1 + p_3}\right)^{(m-y)} .$$

This is the binomial$(m - y, p_1/(p_1 + p_3))$ characteristic function.

For limit theorems of conditional distributions, see Steck (1957)[1] and Holst (1981)[2].

8.3 Problems

1. Derive the characteristic functions for the binomial and the multinomial distributions.

2. Derive the marginal distributions for the multinomial(n, p_1, p_2, p_3, p_4) where $p_1 + p_2 + p_3 + p_4 = 1$.

3. Derive the characteristic function for the Poisson(λ) distribution.

4. For the multivariate normal $\mathcal{N}_n(\mu, \mathbf{\Sigma})$, derive the conditional density

$$f_{X_1, X_2, \ldots X_m | X_{m+1}, \ldots, X_n}(x_1, x_2, \ldots, x_m | x_{m+1}, \ldots, x_n) .$$

[1]Steck, George (1957). *Limit Theorems for Conditional Distributions.* University of California Publications in Statistics **2** 235-284

[2]Holst, Lars (1981). Some conditional limit theorems in exponential families. *Annals of Probability* **9**, 818-830.

5. For the trinomial(n, p_1, p_2, p_3), derive the conditional density $f_{X_1|X_2}(x_1|x_2)$.

6. Show that if $f_X(x) = f_X(-x)$ then $h_X(t)$ is real (the complex part vanishes).

7. Show that if $h_X(t) = 1$ for some $t \neq 0$ that X has a discrete lattice distribution $p_X(a + mk) = P(X = a + mk)$, m an integer for appropriate a and $k = 2\pi/t$.

8. Show that if X_1, X_2 are independent, that $h_{X_1+X_2}(t) = h_{X_1}(t)h_{X_2}(t)$.

9. If X_1 is binomial(n_1, p) and X_2 binomial(n_2, p) and independent, give the distribution of $X_1 + X_2$.

10. If X_1 is negative binomial(r_1, p) and X_2 is negative binomial(r_2, p) and independent, give the distribution of $X_1 + X_2$.

11. If X_1 is Poisson(λ_1) and X_2 Poisson(λ_2) and independent, give the distribution of $X_1 + X_2$.

12. Let $(X, Y) : \mathcal{N}_2((\mu, \eta), \begin{pmatrix} \sigma^2 & \rho\sigma\tau \\ \rho\sigma\tau & \tau^2 \end{pmatrix})$. Using the bivariate characteristic function, calculate $E(X)$, $E(Y)$, $Var(X)$, $Var(Y)$, $Cov(X, Y) = E(XY) - E(X)E(Y)$.

Chapter 9

Asymptotics

9.1 Random Variable Convergences

Definition 9.1 *We say a sequence of random variables* $\{X_n : n = 1, 2, \ldots\}$ *converges in distribution to a random variable* X *and write* $X_n \xrightarrow{d} X$ *if the probability distribution* $F_{X_n}(x)$ *converges to* $F_X(x)$ *for all continuity points* x *of* $F_X(x)$*. In this case, we say* F_{X_n} *converges weakly to* F_X *and write* $F_{X_n} \overset{w}{\Longrightarrow} F_X$*. If* $F_{X_n} \overset{w}{\Longrightarrow} F_X$ *and* $F_{X_n}(\pm\infty) \to F_X(\pm\infty)$ *we say* F_{X_n} *converges completely to* F_X *and write* $F_{X_n} \overset{c}{\Longrightarrow} F_X$*.*

Definition 9.2 *We say a sequence of Borel measurable random variables* $\{X_n : n = 1, 2, \ldots\}$ *on* $(\Omega, \mathcal{A}, P)$ *converges in probability to a random variable* X *and write* $X_n \xrightarrow{p} X$ *if*

$$P(|X_n - X| > \varepsilon) \longrightarrow 0 \text{ as } n \longrightarrow \infty$$

for any $\varepsilon > 0$*.*

Definition 9.3 *We say a sequence of Borel measurable random variables* $\{X_n : n = 1, 2, \ldots\}$ *on* $(\Omega, \mathcal{A}, P)$ *converges almost surely to a random variable* X *and write* $X_n \xrightarrow{a.s.} X$ *if*

$$P(\bigcup_{m=n}^{\infty} \{|X_m - X| > \varepsilon\}) \longrightarrow 0 \text{ as } n \to \infty \text{ for any } \varepsilon > 0 \ .$$

Theorem 9.1 *If* $A = \{\omega : X_n(\omega) \not\to X(\omega)\}$*, then*

$$X_n \xrightarrow{a.s.} X \Longrightarrow P(A) = 0 \ .$$

Proof
Let

$$B_{n\delta} = \{\omega : |X_n(\omega) - X(\omega)| \geq \delta\}, \quad B_\delta = \bigcap_{n=1}^{\infty} \bigcup_{k=n}^{\infty} B_{k\delta} \ .$$

We have

$$\bigcup_{k=n}^{\infty} B_{k\delta} \downarrow B_\delta \text{ and } P(\bigcup_{k=n}^{\infty} B_{k\delta}) \to P(B_\delta) \ .$$

Now

$$A = \{\omega : X_n(\omega) \not\to X(\omega)\} = \bigcup_{\delta>0} B_\delta = \bigcup_{m=1}^{\infty} B_{1/m}$$

since if $\omega \in \bigcup_{\delta>0} B_\delta$, then $\omega \in B_\delta$ for some δ and hence $\omega \in B_{1/m}$ for $1/m < \delta$ and $\omega \in \bigcup_{m=1}^{\infty} B_{1/m}$.
Thus if $X_n \xrightarrow{a.s.} X$ we have $P(\bigcup_{k=n}^{\infty} B_{k\delta}) \to 0$ as $n \to \infty$ and

$$P(B_\delta) = \lim_n P(\bigcup_{k=n}^{\infty} B_{k\delta}) = 0 \text{ and } P(\bigcup_{m=1}^{\infty} B_{1/m}) \leq \sum_{m=1}^{\infty} P(B_{1/m}) = 0 \ . \blacksquare$$

Definition 9.4 *We say a sequence of random variables $\{X_n : n = 1, 2, \ldots\}$ converges in the r-th mean to a random variable X and write $X_n \xrightarrow{r} X$ if*

$$E(|X_n - X|^r) \longrightarrow 0 \text{ as } n \longrightarrow \infty \ .$$

We have the following:

Theorem 9.2 *Almost sure convergence implies convergence in probability implies convergence in distribution:*

$$X_n \xrightarrow{a.s.} X \Longrightarrow X_n \xrightarrow{p} X \Longrightarrow X_n \xrightarrow{d} X \ .$$

Also, convergence in the r-th mean implies convergence in probability:

$$X_n \xrightarrow{r} X \Longrightarrow X_n \xrightarrow{p} X \Longrightarrow X_n \xrightarrow{d} X \ .$$

Proof
$X_n \xrightarrow{a.s.} X \Longrightarrow X_n \xrightarrow{p} X$:

$$P(|X_n - X| > \varepsilon) \leq P(\bigcup_{m=n}^{\infty} \{|X_m - X| > \varepsilon\}) \longrightarrow 0 \ .$$

$X_n \xrightarrow{p} X \Longrightarrow X_n \xrightarrow{d} X$:
Let x be a continuity point of F_X ($x \in C(F_X)$).
If $X_n > x$ and $X - X_n \geq -\varepsilon$ then $X > x - \varepsilon$. Consequently

$$P([X_n > x] \cap [X - X_n > -\varepsilon]) \leq P(X > x - \varepsilon) \ .$$

Taking complements

$$P(X \leq x-\varepsilon) \leq P([X_n \leq x] \cup [X-X_n \leq -\varepsilon]) \leq P(X_n \leq x)+P(|X_n-X| \geq \varepsilon) \ .$$

Similarly, if $X > x + \varepsilon$ and $X_n - X \geq -\varepsilon$ then $X_n > x$ and

$$P([X > x + \varepsilon] \cap [X_n - X > -\varepsilon]) \leq P(X_n > x) \ .$$

Taking complements,

$$P(X_n \leq x) \leq P([X \leq x+\varepsilon] \cup [X_n-X \leq -\varepsilon]) \leq P(X \leq x+\varepsilon)+P(|X_n-X| \geq \varepsilon) \ .$$

Combining these inequalities, we get

$$P(X \leq x-\varepsilon)-P(|X_n-X| \geq \varepsilon) \leq P(X_n \leq x) \leq P(X \leq x+\varepsilon)+P(|X_n-X| \geq \varepsilon) \ .$$

As $n \to \infty$, $P(|X_n - X| \geq \varepsilon) \longrightarrow 0$ and then letting $\varepsilon \to 0$ gives

$$P(X < x) \leq \liminf_n P(X_n \leq x) \leq \limsup_n P(X_n \leq x) \leq P(X \leq x)$$

and $F_{X_n}(x) = P(X_n \leq x) \longrightarrow P(X \leq x) = F_X(x)$ since $P(X = x) = 0$ because $x \in C(F_X)$.
$X_n \xrightarrow{r} X \Longrightarrow X_n \xrightarrow{p} X$:
Markov's inequality is $P(|Y| \geq a) \leq E(|Y|^r)/a^r$. Setting $Y = X_n - X$ gives $P(|X_n - X| \geq \varepsilon) \leq E(|X_n - X|^r)/\varepsilon^r \longrightarrow 0$ as $n \to \infty$ since $X_n \xrightarrow{r} X$. ∎

Example where $X_n \xrightarrow{a.s.} 0$ but $X_n \not\xrightarrow{r} 0$.
Let P be Lebesgue measure on $\Omega = [0, 1]$, and

$$X_n(\omega) = \begin{cases} e^n & \text{for } 0 \leq \omega \leq 1/n \\ 0 & \text{for } 1/n < \omega \leq 1. \end{cases}$$

Then

$$P(\bigcup_{k=n}^{\infty} \{\omega : |X_k(\omega)| \geq \delta\}) = 1/n \to 0$$

and $X_n \xrightarrow{a.s.} 0$. However,

$$E(|X_n|^r) = e^{nr}/n \to \infty \text{ and } X_n \not\xrightarrow{r} 0 \ .$$

Example where $X_{mn} \xrightarrow{p,\, r} 0$ but $X_{mn} \not\xrightarrow{a.s.} 0$ as $n \to \infty$.
Let P be Lebesgue measure on $\Omega = [0, 1]$, and

$$X_{mn}(\omega) = \begin{cases} 1 & \text{for } (m-1)/n < \omega \leq m/n, \quad m = 1, 2, \ldots, n \\ 0 & \text{elsewhere.} \end{cases}$$

Then $E(|X_{mn}|^r) = (1/n)^r \to 0$ and we have convergence in the r-th mean and probability, but

$$P(\bigcup_{k \geq n} \bigcup_{m=1}^{k} [|X_{mk}| > \varepsilon]) = P((0, 1/n] \cup (1/n, 2/n] \cup \cdots \cup ((n-1)/n, 1]) = 1 \not\to 0$$

and we do not have a.s. convergence.

Theorem 9.3 Helly Bray theorem. *Let $F_n \overset{w}{\Longrightarrow} F$, then*

$$\int_{-\infty}^{\infty} g(x) dF_n(x) \longrightarrow \int_{-\infty}^{\infty} g(x) dF(x)$$

for every bounded continuous function g.

Proof.
Assume $|g(x)| \leq c$ and choose $a < b$ such that

$$|\int_{-\infty}^{a} g(x) d(F_n(x) - F(x))| \leq c[F_n(a) + F(a)] < \varepsilon$$

and

$$|\int_{b}^{\infty} g(x) d(F_n(x) - F(x))| \leq c[(1 - F_n(b)) + (1 - F(b))] < \varepsilon \ .$$

Next, partition the interval (a, b) into K intervals using continuity points $x_1, x_2, \ldots, x_{K-1}$ of F where $x_0 = a < x_1 < x_2 < \cdots < x_{K-1} < b = x_K$ are such that

$$|g(x) - g(x_i)| < \varepsilon \text{ for } x_i \leq x < x_{i+1} \ .$$

Define

$$g_K(x) = g(x_i) \text{ for } x_i \leq x < x_{i+1} \ .$$

We have, as $n \to \infty$,

$$\int_a^b g_K(x) dF_n(x) = \sum_{i=0}^{K-1} g(x_i)(F_n(x_{i+1}) - F_n(x_i))$$

$$\longrightarrow \sum_{i=0}^{K-1} g(x_i)(F(x_{i+1}) - F(x_i)) = \int_a^b g_K(x) dF(x)$$

so that for n sufficiently large,

$$|\int_a^b g_K(x) d(F_n(x) - F(x))| < \varepsilon \ .$$

Then

$$|\int_a^b g(x) d(F_n(x) - F(x))|$$

$$= |\int_a^b (g(x) - g_K(x)) dF_n(x) + \int_a^b g_K(x) d(F_n(x) - F(x)) + \int_a^b (g_K(x) - g(x)) dF(x)|$$

$$< \int_a^b \varepsilon dF_n(x) + \varepsilon + \int_a^b \varepsilon dF(x) < 3\varepsilon \ .$$

Combining these results, we have

$$|\int_{-\infty}^{\infty} g(x) d(F_n(x) - F(x))|$$

$$\leq |\int_{-\infty}^{a} g(x) d(F_n(x) - F(x))| + |\int_a^b g(x) d(F_n(x) - F(x))| + |\int_b^{\infty} g(x) d(F_n(x) - F(x))| < 5\varepsilon \ . \blacksquare$$

Theorem 9.4 *Let continuous $g_n(x) \to g(x)$ uniformly in x as $n \to \infty$. If $X_n \stackrel{a.s.}{\to} X$ then $g_n(X_n) \stackrel{a.s.}{\to} g(X)$. If $X_n \stackrel{p}{\to} X$ then $g_n(X_n) \stackrel{p}{\to} g(X)$.*

Proof.
Almost sure convergence follows by a pointwise argument. For convergence in probability, let $\varepsilon > 0$ be given. Then

$$P(|g_n(X_n) - g(X)| \geq \varepsilon) \leq P(|g_n(X_n) - g(X_n)| + |g(X_n) - g(X)| \geq \varepsilon)$$

$$\leq P(|g_n(X_n) - g(X_n)| \geq \varepsilon/2) + P(|g(X_n) - g(X)| \geq \varepsilon/2) \ .$$

Since $g(x)$ is continuous, for any $\delta > 0$, there exists $N_\delta^{(1)}$ so that

$$P(|g(X_n) - g(X)| \geq \varepsilon/2) < \delta/2$$

provided $n \geq N_\delta^{(1)}$ since $X_n \xrightarrow{p} X$. Also since $g_n(x) \to g(x)$ uniformly in x, we have

$$P(|g_n(X_n) - g(X_n)| \geq \varepsilon/2) \leq P(\sup_{X_m} |g_n(X_m) - g(X_m)| \geq \varepsilon/2) < \delta/2$$

for $n \geq N_\delta^{(2)}$. Thus for $n \geq \max\{N_\delta^{(1)}, N_\delta^{(2)}\}$ we have

$$P(|g_n(X_n) - g(X)| \geq \varepsilon) < \delta \ . \blacksquare$$

A useful theorem for proving convergence in distribution is

Theorem 9.5 Continuity Theorem of Paul Lévy
If $F_n(x)$ are distribution functions with characteristic functions $h_n(t)$ such that $\lim_n h_n(t)$ exists for every t and $\lim_n h_n(t) = h(t)$ is continuous at $t = 0$, then there is a distribution function F such that $F_n \to F$ as $n \to \infty$ and h is the characteristic function of F.

Proof.
We first prove a lemma:

Lemma 9.1 *Every sequence of distribution functions contains a subsequence that converges to a function continuous from the right.*

Proof of lemma.
Let $D = \{r_n\}$ be the set of rationals. All terms of the sequence $\{F_n(r_1)\}$ are between 0 and 1. Thus there is a subsequence $\{F_{n_1}(r_1)\}$ that converges. Next for r_2 there is a subsequence $\{n_2\} \subset \{n_1\}$ such that $F_{n_2}(r_2)$ converges. Continuing in this way, we have $F_{n_\nu}(r_k)$ converges for all $r_k \in D$. Let the diagonal sequence

$$c_i = \lim F_{n_i}(r_i) \text{ for } i = 1, 2, \ldots$$

and define

$$F(x) = \inf_{r_i > x} c_i$$

which is continuous from the right. To show that for every x a continuity point of F ($x \in C(F)$) we have

$$F(x) = \lim_{\nu \to \infty} F_{n_\nu}(x) \ .$$

For $x \in C(F)$ we can find a value $\delta > 0$ such that

$$|F(x+\delta) - F(x-\delta)| < \varepsilon \ .$$

Let $r_i < r_k$ be rationals such that

$$x - \delta < r_i < x < r_k < x + \delta \ .$$

Then

$$F(x-\delta) \le c_i \le F(x) \le c_k \le F(x+\delta) \ .$$

Furthur,

$$F_{n_\nu}(r_i) \le F_{n_\nu}(x) \le F_{n_\nu}(r_k)$$

and letting $\nu \to \infty$

$$c_i \le \lim_{\nu} F_{n_\nu}(x) \le c_k \ .$$

Consequently,

$$|\lim_{\nu} F_{n_\nu}(x) - F(x)| < \varepsilon$$

and letting $\varepsilon \to 0$ gives

$$\lim_{\nu} F_{n_\nu}(x) = F(x) \ . \blacksquare$$

Now to prove the theorem it remains to show $F(\infty) - F(-\infty) = 1$ which implies $F(-\infty) = 0$ and $F(\infty) = 1$. From the uniqueness theorem for characteristic functions

$$F_{n_\nu}(x+t) - F_{n_\nu}(x-t) = \lim_{u \to \infty} \frac{1}{2\pi} \int_{-u}^{u} \frac{(e^{-iu(x-t)} - e^{-iu(x+t)})}{iu} h_{n_\nu}(u) du \ .$$

Then

$$\int_0^a (F_{n_\nu}(x+t) - F_{n_\nu}(x-t)) dt = \lim_{u \to \infty} \frac{1}{2\pi} \int_{-u}^{u} \int_0^a \frac{(e^{-iu(x-t)} - e^{-iu(x+t)})}{iu} h_{n_\nu}(u) dt du$$

$$= \lim_{u \to \infty} \frac{1}{2\pi} \int_{-u}^{u} \frac{2(1-\cos(ua))}{u^2} e^{-iux} h_{n_\nu}(u) du \ .$$

Setting $x = 0$ gives

$$\int_0^a (F_{n_\nu}(t) - F_{n_\nu}(-t))dt = \lim_{u\to\infty} \frac{1}{\pi} \int_{-u}^{u} \frac{(1-\cos(ua))}{u^2} h_{n_\nu}(u)du \ .$$

Letting $n_\nu \to \infty$ and dividing by a we get

$$\frac{1}{a}\int_0^a (F(t) - F(-t))dt = \lim_{u\to\infty} \frac{1}{\pi a} \int_{-u}^{u} \frac{(1-\cos(ua))}{u^2} h(u)du$$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{(1-\cos(t))}{t^2} h(t/a)dt \ .$$

Letting $a \to \infty$ using the continuity of $h(t)$ at $t = 0$, gives

$$F(\infty) - F(-\infty) = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{(1-\cos(t))}{t^2} dt = 1.$$

Note

$$F(w)\frac{(a-w)}{a} \le \frac{1}{a}\int_w^a F(t)dt \le \frac{1}{a}\int_0^a F(t)dt \le F(a)$$

and letting $a \to \infty$ gives

$$F(w) \le \lim_{a\to\infty} \frac{1}{a}\int_0^a F(t)dt \le F(\infty) \ .$$

Now let $w \to \infty$ to get

$$\lim_{a\to\infty} \frac{1}{a}\int_0^a F(t)dt = F(\infty) \ .$$

Similarly,

$$\lim_{a\to\infty} \frac{1}{a}\int_0^a F(-t)dt = F(-\infty) \ .$$

Now consider another convergent subsequence of $\{F_n(x)\}$ and denote the limit of the new subsequence by $F^*(x)$. Applying the previous proof, the characteristic functions of the new subsequence have the same limit $h(t)$. By the inversion theorem, and the consequent uniqueness, we have $F^*(x) = F(x)$ for all x. Thus every convergent ubsequence of $\{F_n(x)\}$ has the same limit $F(x)$ which is the c.d.f.$\blacksquare$

Theorem 9.6 *If $X_n \xrightarrow{d} X$ and $g(x)$ is continuous, then $g(X_n) \xrightarrow{d} g(X)$.*

Proof. Writing the characteristic function for $g(X_n)$ and using the Helly-Bray theorem (9.3) on the bounded continuous real and imaginary parts of $e^{itg(x)}$,

$$E(e^{itg(X_n)}) = \int_{-\infty}^{\infty} e^{itg(x)} dF_n(x) \longrightarrow \int_{-\infty}^{\infty} e^{itg(x)} dF(x) = E(e^{itg(X)}) \ .$$

Using Paul Lévy's continuity theorem (9.5) gives the result. ∎

9.2 Laws of Large Numbers.

Theorem 9.7 Borel Cantelli Lemma.
If $\sum_n P(A_n)$ converges, then

$$P(\bigcap_{n=1}^{\infty} \bigcup_{k=n}^{\infty} A_k) = P(\limsup_n A_n) = 0 \ .$$

Proof.

$$[\limsup_n A_n] \subset \bigcup_{k=m}^{\infty} A_k \Longrightarrow P(\limsup_n A_n) \leq P(\bigcup_{k=m}^{\infty} A_k) \leq \sum_{k=m}^{\infty} P(A_k) \to 0$$

as $m \to \infty$ since $\sum_n P(A_n)$ converges.∎

Theorem 9.8 Kolmogorov's Inequality.
Let $X_1, X_2, \ldots, X_n$ be independent with $E(X_i) = 0$ and $Var(X_i) = \sigma_i^2 < \infty$. If $S_n = \sum_{i=1}^n X_i$, then for $\varepsilon > 0$,

$$P(\max_{1 \leq k \leq n} |S_k| \geq \varepsilon) \leq \frac{Var(S_n)}{\varepsilon^2} \ .$$

Proof.
Let the event

$$A_k = \{\omega : |S_k(\omega)| \geq \varepsilon, |S_j(\omega)| < \varepsilon \text{ for } j < k\} \ .$$

The A_k are disjoint and

$$E(S_n^2) \geq \sum_{k=1}^{n} \int_{A_k} S_n^2 dP = \sum_{k=1}^{n} \int_{A_k} (S_k^2 + 2S_k(\sum_{j=k+1}^{n} X_j) + (\sum_{j=k+1}^{n} X_j)^2) dP \ .$$

Since, by independence, $E(S_k I_{A_k} X_j) = E(S_k I_{A_k})E(X_j) = 0$ for $j > k$,

$$Var(S_n) = E(S_n^2) \geq \sum_{k=1}^{n} \int_{A_k} S_k^2 dP \geq \sum_{k=1}^{n} \varepsilon^2 P(A_k) = \varepsilon^2 P(\max_{1\leq k\leq n} |S_k| \geq \varepsilon) \ . \blacksquare$$

Theorem 9.9 Toeplitz Lemma
If a_{nk} $k = 1, 2, \ldots, k_n$ satisfy $a_{nk} \to 0$ for every fixed k and $\sum_k |a_{nk}| \leq c < \infty$, then $x_n \to 0$ gives $s_n = \sum_k a_{nk} x_k \to 0$. If $\sum_k a_{nk} \to 1$ then $x_n \to x$ implies $s_n \to x$. If $b_n = \sum_{k=1}^{n} a_k \uparrow \infty$, then $x_n \to x$ finite implies $\sum_{k=1}^{n} a_k x_k / b_n \to x$.

Proof.
If $x_n \to 0$ then for given $\varepsilon > 0$, $n \geq n_\varepsilon$we have $|x_n| < \varepsilon/c$. Then

$$|s_n| \leq \sum_{k\leq n_\varepsilon} |a_{nk} x_k| + \varepsilon \ .$$

Letting $n \to \infty$ and then $\varepsilon \downarrow 0$ gives $s_n \to 0$.
Next

$$s_n = \sum_k a_{nk} x + \sum_k a_{nk}(x_k - x) \to x$$

using the previous part. Finally, setting $a_{nk} = a_k/b_n$ for $k \leq n$ completes the proof.$\blacksquare$

Theorem 9.10 Kolmogorov's Theorem.
Let $\{X_n : n = 1, 2, \ldots, \infty\}$ be independent with $E(X_i) = \mu_i$ and $Var(X_i) = \sigma_i^2$. Then

$$\sum_{i=1}^{\infty} \frac{\sigma_i^2}{i^2} < \infty \Longrightarrow \frac{\sum_{i=1}^{n} X_i}{n} - \frac{\sum_{i=1}^{n} \mu_i}{n} \xrightarrow{a.s.} 0 \ .$$

Proof.
Without loss of generality, assume $\mu_i = 0$ and let $S_n = X_1 + X_2 + \cdots + X_n$. To show

$$P(\bigcup_{k=n}^{\infty} [|S_k|/k > \varepsilon]) \to 0$$

or $P(\limsup_n [|S_n| > n\varepsilon]) = 0$.
Let

$$B_k = \bigcup_{n=2^k}^{2^{k+1}-1} [|S_n| > n\varepsilon] \ .$$

We have

$$B_k \subset \bigcup_{n=1}^{2^{k+1}} [|S_n| > 2^k \varepsilon]$$

and by Kolmogorov's inequality,

$$P(B_k) \leq P(\max_{1 \leq n < 2^{k+1}} [|S_n| > 2^k \varepsilon]) \leq \frac{1}{\varepsilon^2} \sum_{n=1}^{2^{k+1}} \frac{\sigma_n^2}{(2^k)^2} \ .$$

Thus

$$\sum_{k=0}^{\infty} P(B_k) \leq \frac{1}{\varepsilon^2} \sum_{n=1}^{\infty} \sigma_n^2 \sum_{\substack{k: \\ 2^{k+1} \geq n}} \frac{1}{2^{2k}} \ .$$

If we define $a_n = \lceil \log_2(n) \rceil - 1$ then

$$\sum_{\substack{k: \\ 2^{k+1} \geq n}} \frac{1}{2^{2k}} = \frac{1}{2^{2a_n}} \frac{1}{(1 - 1/4)}$$

and since $a_n \geq \log_2(n) - 1$

$$\sum_{k=0}^{\infty} P(B_k) \leq \frac{1}{\varepsilon^2} \sum_{n=1}^{\infty} \sigma_n^2 \frac{1}{2^{2(\log_2(n)-1)}} \frac{4}{3} = \frac{1}{\varepsilon^2} \sum_{n=1}^{\infty} \sigma_n^2 \frac{16}{3n^2} < \infty \ .$$

By the Borel-Cantelli Lemma, $P(\limsup_n B_n) = 0$ and $P(\limsup_n [|S_n| > n\varepsilon]) = 0$.■

Theorem 9.11 Kolmogorov's Strong Law of Large Numbers.
Let $\{X_n : n = 1, 2, \ldots, \infty\}$ be independent, identically distributed, with $E(X_n) = \mu$ where $|\mu| < \infty$. Then

$$\frac{\sum_{k=1}^{n} X_k}{n} \xrightarrow{a.s.} \mu \ .$$

Proof.
By the assumption, $|\mu| < \infty$ gives $E(|X_1|) < \infty$. Let

$$Y_k = X_k I[|X_k| \leq k] = \begin{cases} X_k & \text{for } |X_k| \leq k \\ 0 & \text{for } |X_k| > k \end{cases}$$

If $A_n = [|X_n| \geq n]$ then

$$\sum_n P(X_n \neq Y_n) \leq \sum_n P(A_n) \leq E(|X_1|) < \infty$$

and by the Borel-cantelli lemma,

$$P(\limsup_n [X_n \neq Y_n]) = 0$$

and $\sum_{k=1}^n X_k/n$ and $\sum_{k=1}^n Y_k/n$ have the same a.s. limit. It suffices to show as $n \to \infty$ that

$$\frac{\sum_{k=1}^n Y_k}{n} \xrightarrow{a.s.} \mu \ .$$

By the dominated convergence theorem,

$$E(Y_n) \longrightarrow E(X_1) = \mu$$

and by the Toeplitz lemma, $E(\sum_{k=1}^n Y_k/n) \to \mu$. It remains to prove

$$\sum_{k=1}^n Y_k/n - E(\sum_{k=1}^n Y_k/n) \xrightarrow{a.s.} 0 \ .$$

This follows using Kolmogorov's theorem, since

$$\sum_n \frac{Var(Y_n)}{n^2} \leq \sum_n \frac{E(Y_n^2)}{n^2} = \sum_n E(\frac{X_1^2}{n^2} I[|X_1| < n]) = \sum_n \frac{1}{n^2} \sum_{k=1}^n E(X_1^2 I[k-1 \leq X_1 < k])$$

$$= \sum_{k=1}^\infty \sum_{n=k}^\infty \frac{1}{n^2} E(X_1^2 I[k-1 \leq X_1 < k]) \leq \sum_{k=1}^\infty \frac{2}{k} E(X_1^2 I[k-1 \leq X_1 < k]) \leq 2E(|X_1|) < \infty$$

using the identity $\sum_{n=k}^\infty \frac{1}{n^2} < 2/k$ for $k \geq 1$.■

The following theorem will be useful for proving convergences of estimators.

Theorem 9.12
Herman Rubin's[1] Uniform Strong Law of Large Numbers.
Let $\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}$ be independent, identically distributed random vectors with c.d.f. $F(\mathbf{x})$. Let Θ be a compact subset of R^K and let $g(\mathbf{x}, \theta)$ be measurable in $\mathbf{x} \in \mathcal{X}$ for each $\theta \in \Theta$. Assume

[1]Rubin, Herman (1956). Uniform convergence of random functions with applications to statistics *Annals of Mathematical Statistics* **27**, 200-203.

(a) *there is a function* $G(\mathbf{x})$ *such that for all* $\mathbf{x} \in \mathcal{X}$ *and all* $\theta \in \Theta$

$$|g(\mathbf{x}, \theta)| \leq G(\mathbf{x}), \text{ where } \int_{\mathcal{X}} G(\mathbf{x}) dF(\mathbf{x}) < \infty \ ,$$

(b) *there is an increasing sequence of measurable sets* S_i *such that*

$$P(\mathcal{X} - \bigcup_{i=1}^{\infty} S_i) = 0$$

and for each i, $g(\mathbf{x}, \theta)$ *is* **equicontinuous** *in* θ *for* $\mathbf{x} \in S_i$.
That is for every $\varepsilon > 0$ *there is a* $\delta > 0$ *such that*

$$|g(\mathbf{x}, \theta_1) - g(\mathbf{x}, \theta_2)| < \varepsilon \text{ for } ||\theta_1 - \theta_2|| < \delta$$

where ε *does not depend on* $\mathbf{x} \in S_i$.

Then

$$\frac{1}{n} \sum_{k=1}^{n} g(\mathbf{X}_k, \theta) \xrightarrow{a.s.} \int_{\mathcal{X}} g(\mathbf{x}, \theta) dF(\mathbf{x})$$

uniformly for $\theta \in \Theta$ *and the limit is continuous in* θ.

Proof.
By the dominated convergence theorem 5.5, and assumptions (a) and (b), for any $\varepsilon > 0$ we can choose i sufficiently large so that

$$\int_{\mathcal{X} - S_i} G(\mathbf{x}) dF(\mathbf{x}) < \varepsilon/5 \text{ since } \int G(\mathbf{x}) I_{[\mathcal{X} - S_i]}(\mathbf{x}) dF(\mathbf{x}) \to 0 \text{ as } i \to \infty \ .$$

Define

$$Z_k = \begin{cases} G(\mathbf{X}_k) & \text{for } \mathbf{X}_k \notin S_i \\ 0 & \text{for } \mathbf{X}_k \in S_i \ . \end{cases}$$

Since $g(\mathbf{x}, \theta)$ is equicontinuous in θ for $\mathbf{x} \in S_i$ and Θ is compact, there exists a finite collection of open sets $V_1, V_2, \ldots, V_m$ for which $\Theta \subset \bigcup_{j=1}^{m} V_j$ and a finite set of points $\theta_j \in V_j$ such that for the $\varepsilon > 0$ above (that is independent of $\mathbf{x}$)

$$|g(\mathbf{x}, \theta) - g(\mathbf{x}, \theta_j)| < \varepsilon/4 \text{ for } \theta \in V_j \ .$$

By the strong law of large numbers (theorem 9.8), we can select N_ε sufficiently large so that for any $\delta > 0$

$$P(|\frac{1}{n}\sum_{k=1}^{n} g(\mathbf{X}_k, \theta_j) - \int g(\mathbf{x}, \theta_j) dF(\mathbf{x})| \geq \varepsilon/4 \text{ for some } n \geq N_\varepsilon) < \frac{\delta}{2m}$$

for $j = 1, 2, \ldots, m$ and also

$$P(|\frac{1}{n}\sum_{k=1}^{n} Z_k| > \varepsilon/4 \text{ for some } n \geq N_\varepsilon) < \frac{\delta}{2}$$

since

$$\frac{1}{n}\sum_{k=1}^{n} Z_k \xrightarrow{a.s.} E(Z_k) = \int_{\mathcal{X}-S_i} G(\mathbf{x}) dF(\mathbf{x}) < \frac{\varepsilon}{5} < \frac{\varepsilon}{4} \ .$$

For $\theta \in V_j$

$$|g(\mathbf{X}_k, \theta) - g(\mathbf{X}_k, \theta_j)| < \frac{\varepsilon}{4} + 2Z_k$$

since

$$|g(\mathbf{X}_k, \theta) - g(\mathbf{X}_k, \theta_j)| < \begin{cases} \varepsilon/4 & \text{for } \mathbf{X}_k \in S_i \\ 2G(\mathbf{X}_k) < 2Z_k + \varepsilon/4 & \text{for } \mathbf{X}_k \notin S_i \ . \end{cases}$$

Then

$$P(|\frac{1}{n}\sum_{k=1}^{n} g(\mathbf{X}_k, \theta) - E(g(\mathbf{X}, \theta_j))| \geq \varepsilon \text{ for some } n \geq N_\varepsilon, \text{ some } \theta_j, \theta \in V_j)$$

$$\leq P(|\frac{1}{n}\sum_{k=1}^{n}(g(\mathbf{X}_k, \theta) - g(\mathbf{X}_k, \theta_j))| + |\frac{1}{n}\sum_{k=1}^{n} g(\mathbf{X}_k, \theta_j) - E(g(\mathbf{X}, \theta_j))| \geq \varepsilon$$

$$\text{for some } n \geq N_\varepsilon, \text{ some } \theta_j, \theta \in V_j)$$

$$\leq P(\varepsilon/4 + |\frac{1}{n}\sum_{k=1}^{n} 2Z_k| + |\frac{1}{n}\sum_{k=1}^{n} g(\mathbf{X}_k, \theta_j) - E(g(\mathbf{X}, \theta_j))| \geq \varepsilon$$

$$\text{for some } n \geq N_\varepsilon, \text{ some } \theta_j \in V_j)$$

$$\leq P(|\frac{1}{n}\sum_{k=1}^{n} 2Z_k| + |\frac{1}{n}\sum_{k=1}^{n} g(\mathbf{X}_k, \theta_j) - E(g(\mathbf{X}, \theta_j))| \geq \frac{3\varepsilon}{4}$$

$$\text{for some } n \geq N_\varepsilon, \text{ some } \theta_j \in V_j)$$

$$\leq P(|\frac{1}{n}\sum_{k=1}^{n} Z_k| > \varepsilon/4 \text{ for some } n \geq N_\varepsilon) +$$

$$P(|\frac{1}{n}\sum_{k=1}^{n} g(\mathbf{X}_k, \theta_j) - E(g(\mathbf{X}, \theta_j))| \geq \varepsilon/4 \text{ for some } n \geq N_\varepsilon, \text{ some } \theta_j \in V_j)$$

$$\leq \frac{\delta}{2} + \sum_{j=1}^{m} \frac{\delta}{2m} = \delta \ .$$

Thus $\sum_{k=1}^{n} g(\mathbf{X}_k, \theta)/n$, which is continuous in θ, converges uniformly in θ (since N_ε does not depend on θ). As the limit of a sequence of continuous functions that converge uniformly is continuous, we have the limit of $\sum_{k=1}^{n} g(\mathbf{X}_k, \theta)/n$ is continuous. By the strong law of large numbers, that limit is $E(g(\mathbf{X}, \theta)) = \int_{\mathcal{X}} g(\mathbf{x}, \theta) dF(\mathbf{x})$. ■

9.3 Central Limit Theorems.

Theorem 9.13 Central Limit Theorem for I.I.D. Random Variables. *If $X_1, X_2, \ldots, X_n$ are independent, identically distributed with $E(X_i) = \mu$ and $Var(X_i) = \sigma^2 < \infty$ then as $n \to \infty$,*

$$Z_n = \frac{\sum_{k=1}^{n} X_k - n\mu}{\sigma\sqrt{n}} \xrightarrow{d} Z$$

where $Z : \mathcal{N}(0, 1)$ has the standard normal distribution.

Proof.
Since $\sigma^2 < \infty$ we can use the expansion in theorem 8.1 for the characteristic function to prove convergence in distribution by showing the characteristic function converges to the characteristic function of a standard normal random variable:

$$h_{Z_n}(u) = \prod_{k=1}^{n} h_{(X_k-\mu)/(\sigma\sqrt{n})}(u) = (1 - \frac{\sigma^2}{2n\sigma^2}u^2 + o(u^2/n))^n \to e^{-u^2/2} \ .$$

We now apply Paul Lévy's continuity theorem 9.3. ■

Theorem 9.14 Liapounov's Central Limit Theorem.
If X_i are independent with $E(X_i) = \mu_i$ and $Var(X_i) = \sigma_i^2 < \infty$ then if $\delta > 0$ and

$$\frac{\sum_{k=1}^n E(|X_k|^{2+\delta})}{[(\sum_{i=1}^n \sigma_i^2)^{1/2}]^{2+\delta}} \to 0 \text{ as } n \to \infty$$

we have

$$Z_n = \frac{\sum_{k=1}^n (X_k - \mu_i)}{(\sum_{i=1}^n \sigma_i^2)^{1/2}} \xrightarrow{d} Z$$

where $Z : \mathcal{N}(0,1)$ has the standard normal distribution.

For a proof see Loève[2], pages 287-288.

As an example, if X_n has a binomial(n,p) distribution, then

$$\frac{X_n - np}{\sqrt{np(1-p)}} \xrightarrow{d} Z : \mathcal{N}(0,1)$$

as $n \to \infty$ since we can think of X_n as a sum of independent identically distributed Bernoulli random variables:

$$X_n = \sum_{i=1}^n W_i \text{ where } W_i = \begin{cases} 1 & \text{with probability } p \\ 0 & \text{with probability } 1-p. \end{cases}$$

The following Beery Esseen theorem is useful for applying the normal approximation.

Theorem 9.15 Beery Esseen Normal Approximation Theorem.
If $X_1, X_2, \ldots, X_n$ are independent, $E(X_i) = 0$, with $S_n = \sum_{i=1}^n X_i$, $\sigma_n^2 = Var(S_n)$, $E|X_i|^3 < \infty$ then

$$\left| P\left[\frac{S_n}{\sigma_n} \le x\right] - \Phi(x) \right| \le \frac{K}{\sigma_n^3} \sum_{i=1}^n E|X_i|^3 \ . \tag{9.1}$$

where the constant $K < \infty$.

For a proof, see, for example, Loève (1977)[1], page 300.

[2]M. Loève *Probability Theory I, Fourth Edition* Springer-Verlag 1977.

9.4 Problems.

1. If $X_n \xrightarrow{d} c$ where c is a finite constant, prove that $X_n \xrightarrow{a.s.} c$.

2. If $X_n \xrightarrow{d} X$ then if g is a continuous function $g(X_n) \xrightarrow{d} g(X)$.

3. Let

$$X_k = \begin{cases} k & \text{with probability } 1/2 \\ 0 & \text{with probability } 1/2. \end{cases}$$

Determine constants a_n and b_n and prove that as $n \to \infty$,

$$Z_n = \frac{\sum_{k=1}^n X_k - a_n}{b_n} \xrightarrow{d} Z : \mathcal{N}(0,1)$$

4. If $X_1, X_2, \ldots, X_n$ are independent Cauchy$(0,1)$ random variables, give the distribution for $\bar{X} = \sum_{i=1}^n X_i/n$ as $n \to \infty$ using characteristic functions.

5. If $X_1, X_2, \ldots, X_n$ are independent identically distributed with $\mathrm{Var}(X_i) = \sigma^2 < \infty$, prove that

$$S^2 = \frac{1}{(n-1)} \sum_{i=1}^n (X_i - \bar{X})^2 \xrightarrow{a.s.} \sigma^2 \ .$$

6. Let $X_1, X_2, \ldots, X_n$ be independent Poisson(λ). Determine constants a_n and b_n such that

$$Z_n = \frac{\sum_{i=1}^n X_i - a_n}{b_n} \xrightarrow{d} Z : \mathcal{N}(0,1).$$

Chapter 10

Sampling Theory for Statistics

10.1 Transformations of Variables

10.1.1 The Continuous Case

In the continuous univariate case, to derive the distribution of a random variable obtained by a 1-1 differentiable transformation from another, we can use the change of variable formula for integrals with $U = g(X)$

$$P(X \in A) = \int_{x \in A} f_X(x)dx = \int_{u \in g(A)} f_X(g^{-1}(u)) \left| \frac{\partial g^{-1}(u)}{\partial u} \right| du$$

where $x = g^{-1}(u)$ is the inverse transform and the absolute value takes a (+) sign for a locally increasing transformation and a (-) sign for a locally decreasing transformation to keep the probability nonnegative. Thus

$$f_U(u) = f_X(g^{-1}(u)) \left| \frac{dg^{-1}(u)}{du} \right| .$$

As an example, consider the exponential$(0, 1)$ density $f_X(x) = e^{-x}$ for $x > 0$ and let $U = e^{-X}$. Then

$$f_U(u) = u \left| \frac{\partial(-\ln u)}{\partial u} \right| = u/u = 1$$

for $0 < u < 1$ and 0 elsewhere (the uniform density on $(0, 1)$).

For the bivariate continuous case with 1-1 differentiable transformations we give the intuition behind the formula for the transformation $U = g_1(X, Y),\ V = g_2(X, Y)$

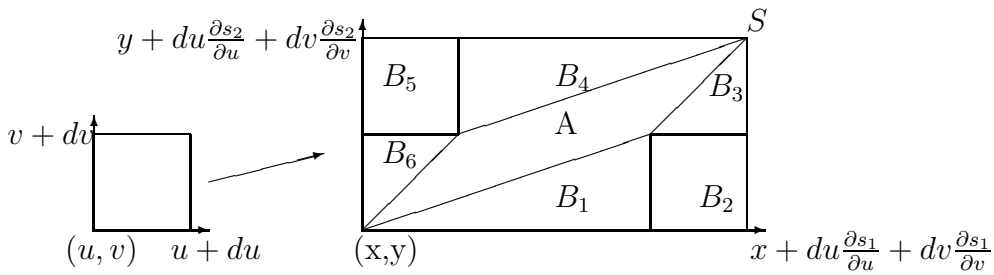

Figure 10.1: Parallelogram illustrating Jacobean calculation.

Consider small values du, dv and

$$P((U,V) \in (u, u+du) \otimes (v, v+dv)) \doteq f_{U,V}(u,v)dudv$$

$$\doteq f_{X,Y}(s_1(u,v), s_2(u,v)) \left\| \begin{matrix} \frac{\partial s_1(u,v)}{\partial u} & \frac{\partial s_1(u,v)}{\partial v} \\ \frac{\partial s_2(u,v)}{\partial u} & \frac{\partial s_2(u,v)}{\partial v} \end{matrix} \right\| dudv$$

where $x = s_1(u,v),\ y = s_2(u,v)$ is the inverse transformation for $u = g_1(x,y),\ v = g_2(x,y)$.

The absolute value of the determinant arises from the transformed area A as illustrated in figure 10.1.

Area $A = S - \sum_{i=1}^{6} B_i$.

Writing

$$s_1(u,v) = x,\ s_2(u,v) = y,$$

$$s_1(u+du, v) \doteq s_1(u,v) + \frac{\partial s_1}{\partial u}du,\ s_2(u+du, v) \doteq s_2(u,v) + \frac{\partial s_2}{\partial u}du,$$

$$s_1(u, v+dv) \doteq s_1(u,v) + \frac{\partial s_1}{\partial v}dv,\ s_2(u, v+dv) \doteq s_2(u,v) + \frac{\partial s_2}{\partial v}dv,$$

$$s_1(u+du, v+dv) \doteq s_1(u,v) + \frac{\partial s_1}{\partial u}du + \frac{\partial s_1}{\partial v}dv,$$

$$s_2(u+du, v+dv) \doteq s_2(u,v) + \frac{\partial s_2}{\partial u}du + \frac{\partial s_2}{\partial v}dv$$

we approximate the transformed area by the parallelogram

$$A = \left(\frac{\partial s_1}{\partial u}du + \frac{\partial s_1}{\partial v}dv\right)\left(\frac{\partial s_2}{\partial u}du + \frac{\partial s_2}{\partial v}dv\right) - \frac{1}{2}\left(\frac{\partial s_1}{\partial u}du\right)\left(\frac{\partial s_2}{\partial u}du\right)$$

$$-\left(\frac{\partial s_2}{\partial u}du\right)\left(\frac{\partial s_1}{\partial v}dv\right) - \frac{1}{2}\left(\frac{\partial s_1}{\partial v}dv\right)\left(\frac{\partial s_2}{\partial v}dv\right) - \frac{1}{2}\left(\frac{\partial s_1}{\partial v}dv\right)\left(\frac{\partial s_2}{\partial v}dv\right)$$

$$-\left(\frac{\partial s_1}{\partial v}dv\right)\left(\frac{\partial s_2}{\partial v}dv\right) - \frac{1}{2}\left(\frac{\partial s_1}{\partial u}du\right)\left(\frac{\partial s_2}{\partial u}du\right)$$

$$= \left(\frac{\partial s_1}{\partial u}\frac{\partial s_2}{\partial v} - \frac{\partial s_1}{\partial v}\frac{\partial s_2}{\partial u}\right)dudv = \begin{vmatrix} \frac{\partial s_1}{\partial u} & \frac{\partial s_1}{\partial v} \\ \frac{\partial s_2}{\partial u} & \frac{\partial s_2}{\partial v} \end{vmatrix} dudv\ .$$

Thus taking the absolute value to insure nonnegative probabilities we have in the limit as $du, dv \to 0$

$$f_{U,V}(u,v) = f_{X,Y}(s_1(u,v), s_2(u,v)) \left\| \begin{matrix} \frac{\partial s_1}{\partial u} & \frac{\partial s_1}{\partial v} \\ \frac{\partial s_2}{\partial u} & \frac{\partial s_2}{\partial v} \end{matrix} \right\|$$

in the 1-1 differentiable case.

For the continuous differentiable multivariate case where the inverse transformations are many to one (say k to 1) the formula extends to

$$f_{U_1,U_2,\ldots,U_n}(\mathbf{u}) = \sum_{i=1}^{k} f_{X_1,X_2,\ldots,X_n}(\mathbf{s^{(i)}}(\mathbf{u})) \left\| \frac{\partial \mathbf{g^{(i)}}}{\partial \mathbf{u}} \right\|$$

where $\mathbf{u} = (u_1, u_2, \ldots, u_n)$, $\mathbf{s^{(i)}}(\mathbf{u}) = (s_1^{(i)}(\mathbf{u}), s_2^{(i)}(\mathbf{u}), \ldots, s_n^{(i)}(\mathbf{u}))$ and

$$\left\| \frac{\partial \mathbf{s^{(i)}}}{\partial \mathbf{u}} \right\| = \left\| \begin{matrix} \frac{\partial s_1^{(i)}}{\partial u_1} & \frac{\partial s_1^{(i)}}{\partial u_2} & \cdots & \frac{\partial s_1^{(i)}}{\partial u_n} \\ \frac{\partial s_2^{(i)}}{\partial u_1} & \frac{\partial s_2^{(i)}}{\partial u_2} & \cdots & \frac{\partial s_2^{(i)}}{\partial u_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial s_n^{(i)}}{\partial u_1} & \frac{\partial s_n^{(i)}}{\partial u_2} & \cdots & \frac{\partial s_n^{(i)}}{\partial u_n} \end{matrix} \right\|$$

is the absolute value of the determinant of the Jacobean for the ith inverse n dimensional transformation.

We note that the inverse can have different multiplicities in different regions. For example, consider the uniform density on the unit square:

$$f_{X,Y}(x,y) = \begin{cases} 1 & \text{for } 0 < x, y < 1 \\ 0 & \text{elsewhere} \end{cases}$$

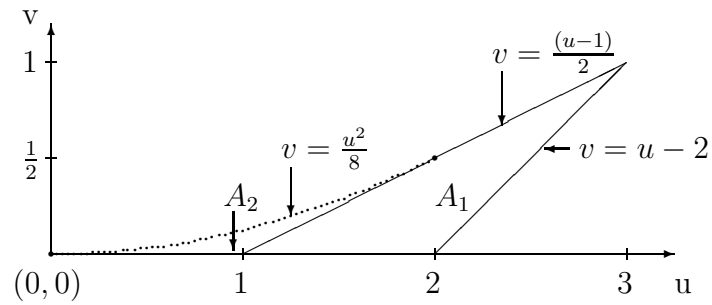

Figure 10.2: Region A_2 of 2-1 inverse transform and region A_1 of 1-1 inverse transform.

and let $U = X + 2Y$, $V = XY$. Then

$$x = s_1^{(1)}(u,v) = \frac{u + \sqrt{u^2 - 8v}}{2}, \quad y = s_2^{(1)}(u,v) = \frac{u - \sqrt{u^2 - 8v}}{4}$$

$$x = s_1^{(2)}(u,v) = \frac{u - \sqrt{u^2 - 8v}}{2}, \quad y = s_2^{(2)}(u,v) = \frac{u + \sqrt{u^2 - 8v}}{4} .$$

Using $s_1^{(1)} \le 1$ and the values are not imaginary gives the region $A_2 =$

$$\{(u,v) \ : \ u^2 \ge 8v, \ u \le 2v + 1, \ \ v \le 1/2\} .$$

Also $s_1^{(2)} \le 1$ and $s_2^{(2)} \le 1$ gives the region $A_1 \cup A_2 =$

$$\{(u,v) \ : \ u^2 \ge 8v \ \& \ 0 < v < 1/2, \ u \ge 2v{+}1 \ \& \ v \ge 1/2, \ u \le v{+}2 \ \& \ 0 < v < 1\} .$$

Then calculating both Jacobeans of the inverse transforms to be $1/\sqrt{u^2 - 8v}$ we have

$$f_{U,V}(u,v) = \begin{cases} \frac{2}{\sqrt{u^2-8v}} & \text{for } (u,v) \in A_2 = \{(u,v) \ : \ \sqrt{8v} \le u \le 2v+1, \ 0 < v < 1/2\} \\ \frac{1}{\sqrt{u^2-8v}} & \text{for } (u,v) \in A_1 = \{(u,v) \ : \ 0 < v < 1, \ 2v+1 \le u \le v+2\} \end{cases} .$$

For an example with many inverse transformations let X_1, X_2, X_3 be independent normal $\mathcal{N}(0, \sigma^2)$ and

$$U_1 = \frac{X_1^2}{X_1^2 + X_2^2}, \quad U_2 = \frac{X_1^2 + X_2^2}{X_1^2 + X_2^2 + X_3^2}, \quad U_3 = X_1^2 + X_2^2 + X_3^2 .$$

There are 8 inverse transformations

$$X_1 = \pm\sqrt{U_1U_2U_3}, \quad X_2 = \pm\sqrt{(1-U_1)U_2U_3}, \quad X_3 = \pm\sqrt{(1-U_2)U_3}$$

corresponding to all 8 possible sign assignments. The joint density is then

$$f_{U_1,U_2,U_3}(u_1,u_2,u_3) = \sum_{i=1}^{8} f_{\mathbf{X}}(\mathbf{s}^{(\mathbf{i})}) \left|\left| \frac{\partial \mathbf{s}^{(\mathbf{i})}}{\partial \mathbf{u}} \right|\right|$$

where the Jacobean of the first inverse transformation $s^{(1)}$ (all + signs) is

$$\left|\left| \frac{\partial \mathbf{s}^{(\mathbf{1})}}{\partial \mathbf{u}} \right|\right| = \left|\left| \begin{array}{ccc} \frac{1}{2}(u_2u_3/u_1)^{1/2} & \frac{1}{2}(u_1u_3/u_2)^{1/2} & \frac{1}{2}(u_1u_2/u_3)^{1/2} \\ -\frac{1}{2}(u_2u_3/(1-u_1))^{1/2} & \frac{1}{2}((1-u_1)u_3/u_2)^{1/2} & \frac{1}{2}((1-u_1)u_2/u_3)^{1/2} \\ 0 & -\frac{1}{2}(u_3/(1-u_2))^{1/2} & \frac{1}{2}((1-u_2)/u_3)^{1/2} \end{array} \right|\right|$$

$$= \frac{\sqrt{u_3}}{8\sqrt{u_1(1-u_1)(1-u_2)}}$$

and is the same for the other 7 transformations. Then

$$f_{U_1,U_2,U_3}(u_1,u_2,u_3) = \frac{8}{(2\pi\sigma^2)^{3/2}} e^{-u_3/(2\sigma^2)} \frac{\sqrt{u_3}}{8\sqrt{u_1(1-u_1)(1-u_2)}}$$

$$= \left(\frac{\Gamma(1)u_1^{1/2-1}(1-u_1)^{1/2-1}}{\Gamma(1/2)\Gamma(1/2)} \right) \left(\frac{\Gamma(3/2)u_2^{1-1}(1-u_2)^{1/2-1}}{\Gamma(1)\Gamma(1/2)} \right) \left(\frac{u_3^{3/2-1}e^{-u_3/(2\sigma^2)}}{\Gamma(3/2)(2\sigma^2)^{3/2}} \right)$$

which is the product of a beta$(1/2, 1/2)$, beta$(1, 1/2)$ and gamma$(3/2, 2\sigma^2)$, density so that U_1, U_2, U_3 are statistically independent. The gamma$(3/2, 2\sigma^2)$ is also called the $\sigma^2\chi^2_3$ density.

An often useful way to calculate the Jacobean of the inverse transformation is to calculate the Jacobean of the direct transform $\mathbf{U} = \mathbf{g}(\mathbf{X})$ evaluated at the inverse and then take the recriprocal of the determinant's absolute value:

$$\left|\left| \frac{\partial \mathbf{s}^{(\mathbf{i})}(\mathbf{u})}{\partial \mathbf{u}} \right|\right| = \left|\left| \begin{array}{cccc} \frac{\partial s_1^{(i)}}{\partial u_1} & \frac{\partial s_1^{(i)}}{\partial u_2} & \cdots & \frac{\partial s_1^{(i)}}{\partial u_n} \\ \frac{\partial s_2^{(i)}}{\partial u_1} & \frac{\partial s_2^{(i)}}{\partial u_2} & \cdots & \frac{\partial s_2^{(i)}}{\partial u_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial s_n^{(i)}}{\partial u_1} & \frac{\partial s_n^{(i)}}{\partial u_2} & \cdots & \frac{\partial s_n^{(i)}}{\partial u_n} \end{array} \right|\right| =$$

$$\left|\left|\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}}\right|\right|^{-1}_{\mathbf{x}=\mathbf{s}^{(\mathbf{i})}(\mathbf{u})} = \left|\left| \begin{array}{cccc} \frac{\partial g_1(x)}{\partial x_1} & \frac{\partial g_1(x)}{\partial x_2} & \cdots & \frac{\partial g_1(x)}{\partial x_n} \\ \frac{\partial g_2(x)}{\partial x_1} & \frac{\partial g_2(x)}{\partial x_2} & \cdots & \frac{\partial g_2(x)}{\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial g_n(x)}{\partial x_1} & \frac{\partial g_n(x)}{\partial x_2} & \cdots & \frac{\partial g_n(x)}{\partial x_n} \end{array} \right|\right|^{-1}_{\mathbf{x}=\mathbf{s}^{(\mathbf{i})}} .$$

The proof uses the chain rule for differentiation. $\mathbf{I_n}$ is the $n \times n$ identity matrix.

$$\mathbf{I_n} = \frac{\partial \mathbf{u}}{\partial \mathbf{u^T}} = \left(\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{u^T}}\right)_{\mathbf{x}=\mathbf{s}(\mathbf{u})} = \left(\left(\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x^T}}\right)\left(\frac{\partial \mathbf{x}}{\partial \mathbf{u^T}}\right)\right)_{\mathbf{x}=\mathbf{s}(\mathbf{u})} = \left(\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x^T}}\right)_{\mathbf{x}=\mathbf{s}(\mathbf{u})}\left(\frac{\partial \mathbf{s}(\mathbf{u})}{\partial \mathbf{u^T}}\right) .$$

Taking the absolute value of the determinant, using the determinant of the product matrix is the product of the matrix determinants, and $||\mathbf{I_n}|| = 1$

$$1 = \left|\left|\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x^T}}\right|\right|_{\mathbf{x}=\mathbf{s}(\mathbf{u})} \left|\left|\frac{\partial \mathbf{s}(\mathbf{u})}{\partial \mathbf{u^T}}\right|\right| . \blacksquare$$

As an example consider the transform $U = X/Y$, $V = X^2 + Y^2$. The Jacobean of the first inverse transform (+sign)

$$s_1^{(1)}(u,v) = \sqrt{\frac{v}{1+u^2}}, \quad s_2^{(1)} = u\sqrt{\frac{v}{1+u^2}}$$

is

$$\left|\left| \begin{array}{cc} \frac{v^{1/2}}{(1+u^2)^{3/2}} & \frac{uv^{-1/2}}{2\sqrt{1+u^2}} \\ \frac{-uv^{1/2}}{(1+u^2)^{3/2}} & \frac{v^{-1/2}}{2\sqrt{1+u^2}} \end{array} \right|\right| = \frac{1}{2(1+u^2)}$$

The Jacobean of the direct transform is

$$\left|\left| \begin{array}{cc} y^{-1} & -xy^{-2} \\ 2x & 2y \end{array} \right|\right| = 2(1+\frac{x^2}{y^2}) .$$

Taking the recriprocal after substituting $\mathbf{s^{(1)}}$ gives $1/(2(1+u^2))$ also but with less difficulty.

10.1.2 The Discrete Case

For transformations of discrete random variables, we simply substitute in the 1-1 case:

$$f_{\mathbf{U}}(\mathbf{u}) = f_{\mathbf{X}}(\mathbf{s}(\mathbf{u})) .$$

For inverse transformations with k to 1 multiplicity we sum over the inverse transforms:

$$f_{\mathbf{U}}(\mathbf{u}) = \sum_{i=1}^{k} f_{\mathbf{X}}(\mathbf{s}^{(\mathbf{i})}(\mathbf{u})) \ .$$

Consider the discrete example with X, Y independent geometric(p):

$$f_{X,Y}(x,y) = p^2 q^{x+y} \text{ where } 0 < q = 1-p < 1$$

and $U = \min\{X,Y\}$, $V = \max\{X,Y\}$. For $u < v$ the inverse transform is 2-1 and for $u = v$ it is 1-1. We have

$$f_{U,V}(u,v) = \begin{cases} 2p^2 q^{u+v} & \text{for } u = 0,1,2,\ldots,v-1 \\ p^2 q^{2v} & \text{for } u = v \end{cases} \quad v = 0,1,2,\ldots,\infty \ .$$

The marginals, obtained by summing, are

$$f_U(u) = q^{2u}(1-q^2), \quad f_V(v) = 2pq^v(1-q^v) + p^2 q^{2v} = (1-q^{v+1})^2 - (1-q^v)^2 \ .$$

10.2 Order Statistics

The order statistics $X_{(1)}, X_{(2)}, \ldots, X_{(n)}$ where $X_{(1)} < X_{(2)} < \cdots < X_{(n)}$ are the sorted values of $X_1, X_2, \ldots, X_n$. If X_i are independent with c.d.f. $F(x)$ and continuous density $f(x)$, then the joint density is

$$f_{X_{(1)},X_{(2)},\ldots,X_{(n)}}(x_{(1)}, x_{(2)}, \ldots, x_{(n)}) = \begin{cases} n! \prod_{i=1}^{n} f(x_{(i)}) & \text{for } x_{(1)} < x_{(2)} < \cdots < x_{(n)} \\ 0 & \text{otherwise} \end{cases}$$

using the $n!$ multiplicity of the inverse transforms with Jacobeans 1 (the determinant of a permutation matrix). If $j_1 < j_2 < \cdots < j_k$, where $j_i \in \{1,2,\ldots,n\}$, then the marginal density

$$f_{X_{(j_1)},X_{(j_2)},\ldots,X_{(j_k)}}(z_1, z_2, \ldots, z_k) = \frac{n! f(z_1) f(z_2) \cdots f(z_k)}{(j_1-1)!(j_2-j_1-1)! \cdots (j_k - j_{k-1} - 1)!(n-j_k)!} \times$$

$$F^{j_1-1}(z_1)(F(z_2)-F(z_1))^{j_2-j_1-1} \cdots (F(z_k)-F(z_{k-1}))^{j_k-j_{k-1}-1}(1-F(z_k))^{n-j_k}$$

for $z_1 < z_2 < \cdots < z_k$, and 0 otherwise. For the transformation $U_{(i)} = F(X_{(i)})$ for $i = 1,2,\ldots,n$ we have

$$f_{U_{(j_1)},U_{(j_2)},\ldots,U_{(j_k)}}(u_1, u_2, \ldots, u_k) = \frac{n!}{(j_1-1)!(j_2-j_1-1)! \cdots (j_k - j_{k-1} - 1)!(n-j_k)!} \times$$

$$u_1^{j_1-1}(u_2-u_1)^{j_2-j_1-1} \cdots (u_k - u_{k-1})^{j_k-j_{k-1}-1}(1-u_k)^{n-j_k} \ .$$

10.3 Linear Transformations

If we have a linear transformation for a continuous distribution

$$U_i = \sum_{j=1}^{n} a_{ij} X_j \text{ for } i = 1, 2, \ldots, n \text{ or in matrix notation } \mathbf{U} = \mathbf{AX}$$

then since this is a 1-1 transformation for $||\mathbf{A}|| > 0$

$$f_{\mathbf{U}}(\mathbf{u}) = \frac{f_{\mathbf{X}}(\mathbf{A^{-1}u})}{||\mathbf{A}||} \ .$$

As a special application, if $\mathbf{X}$ has a multivariate normal $\mathcal{N}_n(\mu, \mathbf{\Sigma})$ density and $\mathbf{U} = \mathbf{AX}$ then

$$f_{\mathbf{U}}(\mathbf{u}) = \frac{e^{-\frac{1}{2}(\mathbf{u^T A^{-T}} - \mu^{\mathbf{T}})\mathbf{\Sigma^{-1}}(\mathbf{A^{-1}u} - \mu)}}{||\mathbf{A}||(2\pi)^{n/2}|\mathbf{\Sigma}|^{1/2}} = \frac{e^{-\frac{1}{2}(\mathbf{u^T} - \mu^{\mathbf{T}}\mathbf{A^T})\mathbf{A^{-T}\Sigma^{-1}A^{-1}}(\mathbf{u} - \mathbf{A}\mu)}}{(2\pi)^{n/2}|\mathbf{A\Sigma A^T}|^{1/2}}$$

where $\mathbf{A^{-T}} = (\mathbf{A^{-1}})^{\mathbf{T}}$ is the transpose of the inverse matrix and $\mathbf{A^{-T}\Sigma^{-1}A^{-1}} = (\mathbf{A\Sigma A^T})^{\mathbf{-1}}$. This is the multivariate normal $\mathcal{N}_n(\mathbf{A}\mu, \mathbf{A\Sigma A^T})$ distribution.

10.4 The Convolution Integral

For X, Y independent with continuous densities, the density of the sum

$$f_{X+Y}(s) = \int_{-\infty}^{\infty} f_X(s-y) f_Y(y) dy \ .$$

Proof.

$$F_{X+Y}(s) = \int_{-\infty}^{\infty} P(X \leq s - y | Y = y) f_Y(y) dy = \int_{-\infty}^{\infty} F_X(s-y) f_Y(y) dy$$

using independence of X, Y. Differentiating under the integral

$$f_{X+Y}(s) = \frac{dF_{X+Y}(s)}{ds} = \int_{-\infty}^{\infty} f_X(s-y) f_Y(y) dy \ . \blacksquare$$

As an application we have the following

Proposition 10.1 *If X_i for $i = 1, 2, \ldots, n$ are independent normal $\mathcal{N}(0, \sigma^2)$ then the density for $U_n = \sum_{i=1}^n X_i^2$ is the $\sigma^2\chi_n^2$ or gamma$(n/2, 2\sigma^2)$ density:*

$$f_{U_n}(s) = \frac{s^{n/2-1}e^{-s/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} \ .$$

Proof.
Using complete induction on n and writing $U_n = U_{n-1} + U_1$ where $U_1 = X_1^2$ and $U_{n-1} = \sum_{i=2}^n X_i^2$

$$f_{U_n}(s) = \int_0^s \frac{(s-y)^{(n-1)/2-1}e^{-(s-y)/(2\sigma^2)}}{\Gamma((n-1)/2)(2\sigma^2)^{(n-1)/2}} \frac{y^{1/2-1}e^{-y/(2\sigma^2)}}{\Gamma(1/2)(2\sigma^2)^{1/2}} dy$$

$$= \frac{s^{n/2-1}e^{-s/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} \int_0^s \frac{\Gamma(n/2)(s-y)^{(n-1)/2-1}y^{1/2-1}}{\Gamma((n-1)/2)\Gamma(1/2)s^{n/2-1}} dy$$

and substituting $v = y/s$

$$= \frac{s^{n/2-1}e^{-s/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} \int_0^1 \frac{\Gamma(n/2)v^{(n-1)/2-1}(1-v)^{1/2-1}}{\Gamma((n-1)/2)\Gamma(1/2)} dv = \frac{s^{n/2-1}e^{-s/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} \times 1$$

using the beta$((n-1)/2, 1/2)$ density integrates to 1. ■

10.5 Distribution of $\bar{X}$ and S^2 for X_i Independent $\mathcal{N}(\mu, \sigma^2)$.

Let $X_1, X_2, \ldots, X_n$ be independent $\mathcal{N}(\mu, \sigma^2)$ and consider

$$\mathbf{Z} = \begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ \vdots \\ Z_n \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \frac{1}{\sqrt{n}} & \cdots & \frac{1}{\sqrt{n}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 & \cdots & 0 \\ \frac{1}{\sqrt{3\cdot 2}} & \frac{1}{\sqrt{3\cdot 2}} & \frac{-2}{\sqrt{3\cdot 2}} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{1}{\sqrt{n\cdot(n-1)}} & \frac{1}{\sqrt{n\cdot(n-1)}} & \frac{1}{\sqrt{n\cdot(n-1)}} & \cdots & \frac{-(n-1)}{\sqrt{n\cdot(n-1)}} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ \vdots \\ X_n \end{pmatrix} .$$

In matrix notation $\mathbf{Z} = \mathbf{AX}$ where A is the above $n \times n$ matrix. We can check that $\mathbf{AA^T} = \mathbf{I_n} = \mathbf{A^TA}$ and

$$\sum_{i=1}^n Z_i^2 = \mathbf{Z^TZ} = \mathbf{X^TA^TAX} = \mathbf{X^TI_nX} = \sum_{i=1}^n X_i^2 \ .$$

Since $\mathbf{X}$ has a multivariate normal $\mathcal{N}_n(\mu\mathbf{1}, \sigma^2\mathbf{I_n})$ distribution where $\mathbf{1} = (1, 1, \ldots, 1)^T$ it follows that $\mathbf{Z}$ has a multivariate normal $\mathcal{N}_n(\boldsymbol{\eta}, \sigma^2\mathbf{I_n})$ since $\sigma^2\mathbf{A}\mathbf{I_n}\mathbf{A^T} = \sigma^2\mathbf{I_n}$ and

$$\boldsymbol{\eta} = \mu\mathbf{A1} = \begin{pmatrix} \mu\sqrt{n} \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}^T .$$

Thus

$$(n-1)S^2 = \sum_{i=1}^n X_i^2 - n\bar{X}^2 = \sum_{i=1}^n Z_i^2 - Z_1^2 = \sum_{i=2}^n Z_i^2$$

has a $\sigma^2\chi^2_{(n-1)}$ distribution since $Z_2, Z_3, \ldots, Z_n$ are independent $\mathcal{N}(0, \sigma^2)$. Also $\sqrt{n}\bar{X} = Z_1$ is independent and $\mathcal{N}(\mu\sqrt{n}, \sigma^2)$. Rescaling, it follows that $\bar{X}$ and S^2 are independent $\mathcal{N}(\mu, \sigma^2/n)$ and $\frac{\sigma^2}{(n-1)}\chi^2_{n-1}$.

10.6 Student's t and Fisher's $\mathcal{F}$ Distribution

Proposition 10.2 *If $Z : \mathcal{N}(0, \sigma^2)$ and $U : \sigma^2\chi^2_n$ are independent, then*

$$T = \frac{Z}{\sqrt{U/n}}$$

has Student's t_n density given by

$$f_T(t) = \frac{\Gamma((n+1)/2)}{(\pi n)^{1/2}\Gamma(n/2)(1 + t^2/n)^{(n+1)/2}} .$$

Proof.

$$f_{T,U}(t, u) = f_{Z,U}(t\sqrt{u/n}, u)||\sqrt{u/n}|| = \frac{e^{-t^2u/(2n\sigma^2)}}{\sigma\sqrt{2\pi}} \frac{u^{n/2-1}e^{-u/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} \sqrt{u/n} .$$

Then

$$f_T(t) = \int_0^\infty f_{T,U}(t, u)du = \int_0^\infty \frac{e^{-t^2u/(2n\sigma^2)}}{\sigma\sqrt{2\pi}} \frac{u^{(n+1)/2-1}e^{-u/(2\sigma^2)}}{\sqrt{n}\Gamma(n/2)(2\sigma^2)^{n/2}} du$$

and letting $v = u(1+t^2/n)/(2\sigma^2)$

$$= \int_0^\infty \frac{e^{-v/2}}{\sigma\sqrt{2n\pi}\Gamma(n/2)(2\sigma^2)^{n/2}} \left(\frac{v2\sigma^2}{(1+t^2/n)}\right)^{(n+1)/2-1} \frac{dv(2\sigma^2)}{(1+t^2/n)}$$

$$= \frac{\Gamma((n+1)/2)}{\sqrt{n\pi}\Gamma(n/2)(1+t^2/n)^{(n+1)/2}} \ . \blacksquare$$

Proposition 10.3 *If $U : \sigma^2\chi^2_m$ and $V : \sigma^2\chi^2_n$ are independent, then*

$$\mathcal{F} = \frac{U/m}{V/n}$$

has Fisher's $\mathcal{F}_{m,n}$ distribution with density

$$f_{\mathcal{F}}(w) = \frac{(m/n)^{m/2}\Gamma((m+n)/2)w^{m/2-1}}{\Gamma(m/2)\Gamma(n/2)(1+wm/n)^{(m+n)/2}}$$

for $0 < w < \infty$.

Proof.

$$f_{\mathcal{F},V}(w,v) = f_{U,V}(wvm/n, v)||vm/n||$$

$$= \frac{(wvm/n)^{m/2-1}e^{-wvm/(n2\sigma^2)}}{\Gamma(m/2)(2\sigma^2)^{m/2}} \frac{v^{n/2-1}e^{-v/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} vm/n \ .$$

Then

$$f_{\mathcal{F}}(w) = \int_0^\infty f_{\mathcal{F},V}(w,v)dv$$

$$= \int_0^\infty \frac{(wvm/n)^{m/2-1}e^{-wvm/(n2\sigma^2)}}{\Gamma(m/2)(2\sigma^2)^{m/2}} \frac{v^{n/2-1}e^{-v/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} vm/ndv$$

and making the change of variable $s = v(1+wm/n)/\sigma^2$

$$= \frac{w^{m/2-1}(m/n)^{m/2}}{(1+wm/n)^{(m+n)/2}} \int_0^\infty \frac{s^{(m+n)/2-1}e^{-s/2}}{\Gamma(m/2)\Gamma(n/2)2^{(m+n)/2}} ds$$

$$= \frac{(m/n)^{m/2}\Gamma((m+n)/2)w^{m/2-1}}{\Gamma(m/2)\Gamma(n/2)(1+wm/n)^{(m+n)/2}} \ . \blacksquare$$

Proposition 10.4 *If $U : \sigma^2\chi^2_m$ and $V : \sigma^2\chi^2_n$ are independent, then*

$$X = \frac{U}{U+V}$$

has the beta$(m/2, n/2)$ density

$$f_X(x) = \frac{\Gamma((m+n)/2)}{\Gamma(m/2)\Gamma(n/2)} x^{m/2-1}(1-x)^{n/2-1} \ .$$

Proof.
For $W = nU/(mV)$ we have $X = (m/n)W/(1+(m/n)W)$ so $W = (n/m)X/(1-X)$ and using the $\mathcal{F}_{m,n}$ density

$$f_X(x) = f_W((n/m)x/(1-x))||(n/m)(1-x)^{-2}||$$

$$= \frac{\Gamma((m+n)/2)}{\Gamma(m/2)\Gamma(n/2)} x^{m/2-1}(1-x)^{n/2-1}(m/n)^{m/2}(n/m)^{m/2} \ . \blacksquare$$

10.7 Noncentral Distributions

Proposition 10.5 *Let X_i be independent normal $\mathcal{N}(\mu_i, \sigma^2)$. The distribution of*

$$U = X_1^2 + X_2^2 + \cdots + X_n^2$$

is the noncentral $\sigma^2\chi^2_n(\delta_n^2/\sigma^2)$ where $\delta_n^2 = \sum_{i=1}^n \mu_i^2$ with density

$$f_U(u) = \sum_{k=0}^{\infty} e^{-\delta_n^2/(2\sigma^2)} \frac{(\delta_n^2/(2\sigma^2))^k}{k!} \frac{u^{(2k+n)/2-1} e^{-u/(2\sigma^2)}}{\Gamma((2k+n)/2)(2\sigma^2)^{(2k+n)/2}}$$

for $u > 0$.

Proof.
Define $\delta_k^2 = \sum_{i=1}^k \mu_i^2$ for $k = 1, 2, \ldots, n$ and set

$$\mathbf{Z} = \begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ \vdots \\ Z_n \end{pmatrix} = \begin{pmatrix} \frac{\mu_1}{\delta_n} & \frac{\mu_2}{\delta_n} & \frac{\mu_3}{\delta_n} & \cdots & \frac{\mu_n}{\delta_n} \\ \frac{\mu_2\mu_1}{\delta_2\delta_1} & \frac{-\delta_1^2}{\delta_2\delta_1} & 0 & \cdots & 0 \\ \frac{\mu_3\mu_1}{\delta_3\delta_2} & \frac{\mu_3\mu_2}{\delta_3\delta_2} & \frac{-\delta_2^2}{\delta_3\delta_2} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\mu_n\mu_1}{\delta_n\delta_{n-1}} & \frac{\mu_n\mu_1}{\delta_n\delta_{n-1}} & \frac{\mu_n\mu_1}{\delta_n\delta_{n-1}} & \cdots & \frac{-\delta_{n-1}^2}{\delta_n\delta_{n-1}} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ \vdots \\ X_n \end{pmatrix} \ .$$

In matrix notation $\mathbf{Z} = \mathbf{AX}$ where $\mathbf{A}$ is the previous $n \times n$ matrix and satisfies $\mathbf{AA^T} = \mathbf{A^TA} = \mathbf{I_n}$. It follows from $\mathbf{X} : \mathcal{N}_n(\mu, \sigma^2\mathbf{I_n})$ where $\boldsymbol{\mu} = (\mu_1, \mu_2, \ldots, \mu_n)^T$ that $\mathbf{Z} : \mathcal{N}_n(\eta, \sigma^2\mathbf{I_n})$ with $\eta = (\delta_n, 0, 0, \ldots, 0)^T$. Also

$$\sum_{i=1}^{n} Z_i^2 = \mathbf{Z^TZ} = \mathbf{X^TA^TAX} = \mathbf{X^TX} = \sum_{i=1}^{n} X_i^2 = U \ .$$

The density

$$\begin{aligned} f_{Z_1^2}(u) &= f_{Z_1}(\sqrt{u}) \left|\left| \frac{d\sqrt{u}}{du} \right|\right| + f_{Z_1}(-\sqrt{u}) \left|\left| \frac{d(-\sqrt{u})}{du} \right|\right| \\ &= \frac{\frac{1}{2}u^{-1/2}e^{(\sqrt{u}-\delta_n)^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}} + \frac{\frac{1}{2}u^{-1/2}e^{(-\sqrt{u}-\delta_n)^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}} \\ &= \frac{u^{1/2-1}e^{-u/(2\sigma^2)}}{\Gamma(1/2)(2\sigma^2)^{1/2}} e^{-\delta_n^2/(2\sigma^2)} \left(\frac{e^{\delta_n\sqrt{u}/\sigma^2} + e^{-\delta_n\sqrt{u}/\sigma^2}}{2} \right) \\ &= \sum_{k=0}^{\infty} e^{-\delta_n^2/(2\sigma^2)} \frac{(\delta_n^2/(2\sigma^2))^k}{k!} \frac{u^{(2k+1)/2-1}e^{-u/(2\sigma^2)}}{\Gamma((2k+1)/2)(2\sigma^2)^{(2k+1)/2}} \ . \end{aligned}$$

Forming the convolution $Z_1^2 + \sum_{i=2}^{n} Z_i^2$ term by term and using the convolution of $\sigma^2\chi^2_{2k+1}$ and $\sigma^2\chi^2_{n-1}$ is $\sigma^2\chi^2_{2k+n}$ gives

$$f_U(u) = f_{\sum_{i=1}^{n} Z_i^2}(u) = \sum_{k=0}^{\infty} e^{-\frac{\delta_n^2}{2\sigma^2}} \frac{\left(\frac{\delta_n^2}{2\sigma^2}\right)^k}{k!} \frac{u^{(2k+n)/2-1}e^{-u/(2\sigma^2)}}{\Gamma((2k+n)/2)(2\sigma^2)^{(2k+n)/2}} \ . \blacksquare$$

Thus the noncentral $\sigma^2\chi_n^2(\delta_n^2/\sigma^2)$ density is a Poisson$(\delta_n^2/(2\sigma^2))$ probability mixture of central $\sigma^2\chi^2_{2k+n}(0)$ densities.

Proposition 10.6 *Let $U : \sigma^2\chi_m(\delta^2)$ and $V : \sigma^2\chi_n^2(0)$ be independent.*

$$W = \frac{U}{U+V}$$

has the noncentral beta$(\delta^2, m/2, n/2)$ density given by

$$f_W(w) = \sum_{k=0}^{\infty} e^{-\frac{\delta^2}{2}} \frac{\left(\frac{\delta^2}{2}\right)^k}{k!} \frac{\Gamma((2k+m+n)/2)}{\Gamma((2k+m)/2)\Gamma(n/2)} w^{(2k+m)/2-1}(1-w)^{n/2-1} \ .$$

Proof.

$$f_{W,V}(w,v) = f_{U,V}(wv/(1-w),v)\left|\frac{v}{(1-w)^2}\right|$$

$$= \sum_{k=0}^{\infty} \frac{e^{-\frac{\delta^2}{2}}\left(\frac{\delta^2}{2}\right)^k}{k!} \frac{\left(\frac{wv}{1-w}\right)^{\frac{2k+m}{2}-1} e^{-\frac{wv}{(1-w)2\sigma^2}}}{\Gamma(\frac{2k+m}{2})(2\sigma^2)^{\frac{2k+m}{2}}} \frac{v^{n/2-1}e^{-v/(2\sigma^2)}}{\Gamma(n/2)(2\sigma^2)^{n/2}} \frac{v}{(1-w)^2}$$

Integrating to obtain the marginal

$$f_W(w) = \int_0^\infty f_{W,V}(w,v)dv =$$

$$\sum_{k=0}^{\infty} \frac{e^{-\frac{\delta^2}{2}}\left(\frac{\delta^2}{2}\right)^k}{k!} \frac{\left(\frac{w}{1-w}\right)^{\frac{2k+m}{2}-1} \frac{1}{(1-w)^2}}{\Gamma(\frac{2k+m}{2})\Gamma(\frac{n}{2})(2\sigma^2)^{\frac{2k+m+n}{2}}} \int_0^\infty v^{\frac{2k+m+n}{2}-1} e^{-\frac{v}{2\sigma^2}(1+\frac{w}{(1-w)})} dv \ .$$

Making the change of variable $t = v/(\sigma^2(1-w))$ gives

$$f_W(w) = \sum_{k=0}^{\infty} \frac{e^{-\frac{\delta^2}{2}}\left(\frac{\delta^2}{2}\right)^k}{k!} \frac{w^{\frac{2k+m}{2}-1}(1-w)^{\frac{n}{2}-1}}{\Gamma(\frac{2k+m}{2})\Gamma(\frac{n}{2})2^{\frac{2k+m+n}{2}}} \int_0^\infty t^{\frac{2k+m+n}{2}-1} e^{-t/2} dt$$

$$= \sum_{k=0}^{\infty} \frac{e^{-\frac{\delta^2}{2}}\left(\frac{\delta^2}{2}\right)^k}{k!} \frac{\Gamma\left(\frac{2k+m+n}{2}\right) w^{\frac{2k+m}{2}-1}(1-w)^{\frac{n}{2}-1}}{\Gamma\left(\frac{2k+m}{2}\right)\Gamma\left(\frac{n}{2}\right)} \ . \blacksquare$$

This is a Poisson$(\delta^2/2)$ probability mixture of beta$((2k+m)/2, n/2)$ densities.

The noncentral $t_n(\delta)$ distribution is defined by

$$T = \frac{Z+\delta}{\sqrt{U/n}}$$

where $Z : \mathcal{N}(0,1)$ and $U : \chi_n^2(0)$ are independent. There seems to be no nice closed form expression for the density. The c.d.f. can be calculated from

$$F_T(t) = \int_0^\infty \Phi(t\sqrt{\frac{u}{n}} - \delta)\frac{u^{n/2-1}e^{-u/2}}{\Gamma(n/2)2^{n/2}}du$$

where $\Phi(x)$ is the c.d.f. for the $\mathcal{N}(0,1)$ distribution.

10.8 Chi square distribution of $\mathbf{X}^T\mathbf{\Sigma}^-\mathbf{X}$

Proposition 10.7 *Let* $\mathbf{X} : \mathcal{N}_K(\mathbf{0}, \mathbf{\Sigma})$ *where* $\mathbf{\Sigma}^{K\times K}$ *is symmetric, positive semidefinate of rank* $r \leq K$*. Then the quadratic form*

$$\mathbf{X}^T\mathbf{\Sigma}^-\mathbf{X}$$

has a noncentral $\chi^2_r(0)$ *distribution where* $\mathbf{\Sigma}^-$ *is a generalized inverse of* $\mathbf{\Sigma}$ *that satisfies* $\mathbf{\Sigma}\mathbf{\Sigma}^-\mathbf{\Sigma} = \mathbf{\Sigma}$*.*

Proof.
Let $\mathbf{A}\mathbf{\Sigma}\mathbf{A}^T = \mathbf{D}$ where $\mathbf{A}$ is $K \times K$ nonsingular, and the diagonal matrix

$$\mathbf{D}^{K\times K} = \begin{pmatrix} \mathbf{I}_r^{r\times r} & \mathbf{0}^{r\times(K-r)} \\ \mathbf{0}^{(K-r)\times r} & \mathbf{0}^{(K-r)\times(K-r)} \end{pmatrix} .$$

$\mathbf{I}_r$ is the $r \times r$ identity matrix and $\mathbf{0}$ is a matrix of zeros. See for example page 344, theorem 6 of Anderson (1958)[1]. Let $\mathbf{\Sigma}_0^- = \mathbf{A}^T\mathbf{D}\mathbf{A}$. Then it is a generalized inverse of $\mathbf{\Sigma}$ using $\mathbf{D}^2 = \mathbf{D}$

$$\mathbf{\Sigma}\mathbf{\Sigma}_0^-\mathbf{\Sigma} = (\mathbf{A}^{-1}\mathbf{D}\mathbf{A}^{-T})(\mathbf{A}^T\mathbf{D}\mathbf{A})(\mathbf{A}^{-1}\mathbf{D}\mathbf{A}^{-T}) = \mathbf{A}^{-1}\mathbf{D}\mathbf{A}^{-T} = \mathbf{\Sigma} .$$

Also, any generalize inverse $\mathbf{\Sigma}^-$ of $\mathbf{\Sigma}$ is of the form

$$\mathbf{\Sigma}^- = \mathbf{\Sigma}_0^- + (\mathbf{W} - \mathbf{\Sigma}_0^-\mathbf{\Sigma}\mathbf{W}\mathbf{\Sigma}\mathbf{\Sigma}_0^-)$$

where $\mathbf{W}^{K\times K}$ is arbitrary, since

$$\mathbf{\Sigma}\mathbf{\Sigma}^-\mathbf{\Sigma} = \mathbf{\Sigma}\mathbf{\Sigma}_0^-\mathbf{\Sigma} + (\mathbf{\Sigma}\mathbf{W}\mathbf{\Sigma} - \mathbf{\Sigma}\mathbf{\Sigma}_0^-\mathbf{\Sigma}\mathbf{W}\mathbf{\Sigma}\mathbf{\Sigma}_0^-\mathbf{\Sigma})$$

$$= \mathbf{\Sigma} + (\mathbf{\Sigma}\mathbf{W}\mathbf{\Sigma} - \mathbf{\Sigma}\mathbf{W}\mathbf{\Sigma}) = \mathbf{\Sigma} .$$

Then

$$\mathbf{X}^T\mathbf{\Sigma}^-\mathbf{X} = \mathbf{X}^T\mathbf{\Sigma}_0^-\mathbf{X} + \mathbf{Z}^T(\mathbf{W} - \mathbf{\Sigma}_0^-\mathbf{\Sigma}\mathbf{W}\mathbf{\Sigma}\mathbf{\Sigma}_0^-)\mathbf{Z} .$$

Let

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}_1^{r\times 1} \\ \mathbf{U}_2^{(K-r)\times 1} \end{pmatrix} = \mathbf{A}\mathbf{X} : \mathcal{N}_K(\mathbf{0}, \mathbf{D})$$

[1] Anderson, T.W. (1958). *An Introduction to Multivariate Statistical Analysis.* John Wiley, New York

so that $\mathbf{U}_1 : \mathcal{N}_r(\mathbf{0}, \mathbf{I}_r)$ and $P(\mathbf{U}_2 = \mathbf{0}) = 1$. Substituting, with $\mathbf{U}$ and

$$\mathbf{A}^{-T}\mathbf{W}\mathbf{A}^{-1} = \mathbf{B}^{K\times K} = \begin{pmatrix} \mathbf{B}_{11}^{r\times r} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{pmatrix}$$

we obtain

$$\mathbf{X}^T\mathbf{\Sigma}^-\mathbf{X} = \mathbf{U}^T\mathbf{A}^{-T}(\mathbf{A}^T\mathbf{D}\mathbf{A})\mathbf{A}^{-1}\mathbf{U} + (\mathbf{U}^T(\mathbf{A}^{-T}\mathbf{W}\mathbf{A}^{-1})\mathbf{U} - \mathbf{U}^T\mathbf{D}(\mathbf{A}^{-T}\mathbf{W}\mathbf{A}^{-1})\mathbf{D}\mathbf{U})$$

$$= \mathbf{U}_1^T\mathbf{U}_1 + (\mathbf{U}^T\mathbf{B}\mathbf{U} - \mathbf{U}^T\mathbf{D}\mathbf{B}\mathbf{D}\mathbf{U})$$

$$= \mathbf{U}_1^T\mathbf{U}_1 + \mathbf{U}_1^T\mathbf{B}_{12}\mathbf{U}_2 + \mathbf{U}_2^T\mathbf{B}_{21}\mathbf{U}_1 + \mathbf{U}_2^T\mathbf{B}_{22}\mathbf{U}_2 = \mathbf{U}_1^T\mathbf{U}_1 : \chi_r^2(0) \ . \quad \blacksquare$$

Proposition 10.8 *Let* $\mathbf{X} : \mathcal{N}_K(\boldsymbol{\mu}, \mathbf{\Sigma})$ *where* $\mathbf{\Sigma}^{K\times K}$ *is symmetric, positive semidefinate of rank* $r \leq K$. *Define* $\mathbf{\Sigma}^-$ *to be a* $K \times K$ *matrix which*

(a) *is a generalized inverse (*$\mathbf{\Sigma}\mathbf{\Sigma}^-\mathbf{\Sigma} = \mathbf{\Sigma}$*),*

(b) *is symmetric (*$\mathbf{\Sigma}^- = (\mathbf{\Sigma}^-)^T$*),*

(c) *is reflexive (*$\mathbf{\Sigma}^-\mathbf{\Sigma}\mathbf{\Sigma}^- = \mathbf{\Sigma}^-$*).*

Then

$$\mathbf{X}^T\mathbf{\Sigma}^-\mathbf{X}$$

has a noncentral $\chi_r^2(\delta^2)$ *distribution, with noncentrality parameter*

$$\delta^2 = \boldsymbol{\mu}^T\mathbf{\Sigma}^-\boldsymbol{\mu} \ .$$

For a proof, see Rao and Mitra (1971)[2], page 173, theorem 9.3.2.

10.9 Problems

1. Let X, Y be independent with continuous density $f(x) = e^{-x}$ for $x > 0$ and 0 elsewhere. Derive the joint density for $U = X+Y$ and $V = X-Y$ and give the marginal densities $f_U(u)$ and $f_V(v)$.

2. Let X_1, X_2 be independent $\mathcal{N}(0, 1)$. Derive the density for $U = X_1/X_2$.

[2]Rao, C. R. and Mitra, S. K. (1971). *Generalized Inverse of Matrices and its Applications.* John Wiley, New York.

3. Let X_i be Bernoulli(p) random variables ($P(X_i = 1) = p = 1 - P(X_i = 0)$ for $0 < p < 1$) . If N:Binomial(n, p), give the discrete density $f_{S,N}(s, k)$ and $f_S(s)$ for the random sum $S = \sum_{i=1}^{N} X_i$

4. Let X_i be independent with discrete density $p_{X_i}(x_i) = q^{x_i - m} p$ for $x_i = m, m+1, m+2, \ldots, \infty$, $q = 1 - p$, $0 < p < 1$. Assume $U = \sum_{i=1}^{n}(X_i - X_{(1)})$ and $V = X_{(1)}$ are independent. Give $f_{U,V}(u, v)$ and $f_U(u)$, $p_V(v)$.

5. Let X, Y be independent with density

$$f(x) = \begin{cases} \frac{\alpha}{x^{\alpha+1}} & \text{for } x \geq 1 \\ 0 & \text{for } x < 1 \end{cases}$$

Derive the density for $U = \sqrt{XY}$.

6. Let $(X, Y) : \mathcal{N}_2((0,0), \sigma^2 \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix})$. Derive the joint density for $U = X + Y$, $V = X - Y$.

7. Let X, Y be independent $\mathcal{N}(0, 1)$.Using the convolution integral, derive the density for $U = X + Y$.

8. Let $\boldsymbol{X}^{K \times 1} : \mathcal{N}_K(\mathbf{0}, \boldsymbol{\Sigma})$ where

$$\boldsymbol{\Sigma} = \begin{pmatrix} \rho_1 & 0 & \cdots & 0 \\ 0 & \rho_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \rho_K \end{pmatrix} - \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_K \end{pmatrix} \begin{pmatrix} \rho_1 , & \rho_2 , & \cdots , & \rho_K \end{pmatrix},$$

$0 < \rho_i$, and $\sum_{i=1}^{K} \rho_i = 1$. Give the distribution of $\sum_{i=1}^{K} \frac{X_i^2}{\rho_i}$.

9. Let $\mathbf{X}^{K\times 1} : \mathcal{N}_K(\boldsymbol{\lambda}, \boldsymbol{\Sigma})$ where

$$\boldsymbol{\lambda} = \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_K \end{pmatrix}, \ \boldsymbol{\Sigma} = \begin{pmatrix} \rho_1 & 0 & \cdots & 0 \\ 0 & \rho_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \rho_K \end{pmatrix} - \begin{pmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_K \end{pmatrix} \begin{pmatrix} \rho_1, & \rho_2, & \cdots, & \rho_K \end{pmatrix},$$

$\lambda_i, \rho_i > 0$ for $i = 1, 2, \ldots, K$, with $\sum_{i=1}^K \lambda_i = 1 = \sum_{i=1}^K \rho_i$.
For

$$\boldsymbol{\Sigma}^- = \begin{pmatrix} 1/\rho_1 & 0 & \cdots & 0 \\ 0 & 1/\rho_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1/\rho_K \end{pmatrix} - \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \begin{pmatrix} 1, & 1, & \cdots, & 1 \end{pmatrix}^{1\times K},$$

(i) Verify conditions (a),(b), and (c) of proposition 10.8.

(ii) Give the distribution of

$$\mathbf{X}^T \boldsymbol{\Sigma}^- \mathbf{X} = \sum_{i=1}^K \left(X_i - \rho_i \sum_{k=1}^K X_k \right)^2 .$$

(iii) What is the distribution if $\lambda_i = \rho_i$ for $i = 1, 2, \ldots, K$?

Chapter 11

Point Estimation

11.1 Sufficient Statistics

For a set of observations $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ it is of interest to find functions of this data that can be used for making inferences about unknown parameters of the distribution.

We consider a family of distributions $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ where θ is a vector of unknown parameters and P_θ is a probability distribution for the data $\mathbf{X}$. The idea of a sufficient statistic $\mathbf{S}(\mathbf{X})$, a function of the data which may be vector valued, is that any inference using the full data set $\mathbf{X}$ can just as well be made using $\mathbf{S}(\mathbf{X})$ provided the family of distributions $\mathcal{P}$ for which $\mathbf{S}(\mathbf{X})$ is sufficient is the correct distribution for $\mathbf{X}$.

Definition 11.1 *We say* $\mathbf{S}(\mathbf{X})$ *is sufficient for* $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ *if for all* $A \in \mathcal{B}^{(n)}$*, the Borel sigma field on* R^n*,*

$$P_\theta(\mathbf{X} \in A | \mathbf{S}(\mathbf{X}) = \mathbf{s})$$

does not depend on θ *for almost every*[1] $\mathbf{s}$*.*

The idea behind this definition is that we can use the conditional distribution which is known, since it does not depend on the unknown parameter θ, to reconstruct another sample with the same distribution as $\mathbf{X}$. Since this reconstructed sample has the same distribution as $\mathbf{X}$, it is equally useful for making statistical inferences.

[1] It holds for every $\mathbf{s}$ except possibly for $\mathbf{s} \in N$ where $P_\theta(N) = 0$ for all $\theta \in \Theta$.

As an example, let X_1, X_2 be independent Poisson(θ) for unknown $\theta \in (0, \infty)$. Consider $S(X_1, X_2) = X_1 + X_2$. We have

$$P(X_1 = x_1, X_2 = s - x_1 | X_1 + X_2 = s) = \frac{\theta^s e^{-2\theta}}{x_1!(s - x_1)!} / \frac{(2\theta)^s e^{-2\theta}}{s!} = \begin{pmatrix} s \\ x_1 \end{pmatrix} \frac{1}{2^s} .$$

Thus the conditional distribution is the binomial($n, 1/2$) distribution and we could reconstruct another sample $X_1^{'}, X_2^{'}$ by tossing a coin s times and letting $X_1^{'}$ be the number of heads and $X_2^{'}$ the number of tails.

To identify the sufficient statistic for a family of distributions we can use

Theorem 11.1 Neyman-Fisher Factorization Theorem. *Let* $\mathbf{X}$ *have a distribution which belongs to* $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ *where* $P_\theta << \mu$ *for all* $\theta \in \Theta$. *Then* $\mathbf{S}(\mathbf{X})$ *is sufficient for* $\mathcal{P}$ *if and only if the joint density is of the form*

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{dP_\theta}{d\mu}(\mathbf{x}) = g(\mathbf{S}(\mathbf{x}), \theta) h(\mathbf{x})$$

where g *depends on* θ *and on* $\mathbf{x}$ *only through the function* $\mathbf{S}(\mathbf{x})$ *and* h *does not depend on* θ.

We first prove a lemma.

Lemma 11.1 *A family* $\mathcal{P}$ *of probability measures satisfies* $P << \mu$ *for all* $P \in \mathcal{P}$ *for some* μ *if and only if there is a countable family* $\{P_i : i = 1, 2, \ldots, \infty\}$, $P_i \in \mathcal{P}$ *such that* $P << \sum_i c_i P_i$ *where* $c_i > 0$, $\sum_i c_i = 1$ *for all* $P \in \mathcal{P}$.

Proof of lemma 11.1.
If such a subset $\{P_i : i = 1, 2, \ldots, \infty\}$ exists take $\mu = \sum_i c_i P_i$.
Conversely, assume $P << \mu$ for all $P \in \mathcal{P}$. To show that there exists such a collection $\{P_i : i = 1, 2, \ldots, \infty\}$.
Define $\mathcal{Q}$ to be the class of all probability measures of the form $Q = \sum_i c_i P_i$ where $P_i \in \mathcal{P}$, $c_i > 0$, and $\sum_i c_i = 1$. $Q << \mu$ implies there exists a density $q(x) = \frac{dQ}{d\mu}(x)$ by the Radon-Nikodym theorem. Since $\mathcal{P} \subset \mathcal{Q}$ it suffices to prove there exists a $Q_0 \in \mathcal{Q}$ such that $Q_0(A) = 0$ implies $Q(A) = 0$ for all $Q \in \mathcal{Q}$
Define the class $\mathcal{C}$ of sets $C \in \mathcal{A}$ for which there exists $Q \in \mathcal{Q}$ such that $q(x) > 0$ a.e.$[\mu]$[2] for $x \in C$ and $Q(C) > 0$. We have $\mathcal{C}$ is not empty since

[2] $q(x) > 0$ for all x except possibly for $x \in D$ where $\mu(D) = 0$.

$1 = Q(\Omega) = \int_{\{x:q(x)>0\}} q(x)d\mu(x) = Q(C)$ where $C = \{x : q(x) > 0\}$.
Let $\mu(C_i) \to \sup_{C\in\mathcal{C}} \mu(C)$. For $C \in \mathcal{C}$, $Q(C) > 0$ and $q(x) > 0$ for $x \in C$ so we have $\mu(C) > 0$, $\sup_{C\in\mathcal{C}} \mu(C) > 0$, and $\mu(C_i) > 0$ for i sufficiently large ($i \geq N$).
Since $C_i \in \mathcal{C}$, $Q_i(C_i) > 0$ for some $Q_i \in \mathcal{Q}$ and $q_i(x) > 0$ a.e. $[\mu]$ for $x \in C_i$.
Denote $C_0 = \bigcup_{i=N}^{\infty} C_i$ and $q_0(x) = \sum_{i=N}^{\infty} c_i q_i(x)$, $Q_0 = \sum_{i=N}^{\infty} c_i Q_i$. We have $Q_0(C_0) > 0$ and $q_0(x) > 0$ a.e. $[\mu]$ for $x \in C_0$ so $C_0 \in \mathcal{C}$.
Suppose $Q_0(A) = 0$ and let Q be any member of $\mathcal{Q}$. To show $Q(A) = 0$.

$$Q_0(A) = 0 \Longrightarrow Q_0(A \cap C_0) = 0 \Longrightarrow \mu(A \cap C_0) = 0 \Longrightarrow Q(A \cap C_0) = 0$$

since $q_0(x) > 0$ for $x \in A \cap C_0 \subset C_0$ and $Q << \mu$.
Next for $C = \{x : q(x) > 0\}$, $Q(A \cap C_0^c \cap C^c) = 0$ since $q(x) = 0$ for $x \in C^c$.
Finally, $Q(A \cap C_0^c \cap C) = 0$ since if not

$$Q(A \cap C_0^c \cap C) > 0 \Longrightarrow \mu(A \cap C_0^c \cap C) > 0 \Longrightarrow \mu(C_0 \cup (A \cap C_0^c \cap C)) > \mu(C_0)$$

which is a contradiction to $\mu(C_0) = \sup_{C\in\mathcal{C}} \mu(C)$ since $A \cap C_0^c \cap C \in \mathcal{C}$ and $C_0 \cup (A \cap C_0^c \cap C) \in \mathcal{C}$
Thus

$$Q(A) = Q(A \cap C_0) + Q(A \cap C_0^c \cap C^c) + Q(A \cap C_0^c \cap C) = 0 + 0 + 0 = 0 \,. \blacksquare$$

Proof of theorem 10.1.
Using lemma 10.1 let $Q_0 = \sum_i c_i P_{\theta_i}$ satisfy $P_\theta(A) = 0$ for all θ if and only if $Q_0(A) = 0$. Suppose S is sufficient for θ. Then for $A_0 \in \mathcal{A}(S(X))$, $A \in \mathcal{A}$ and all θ

$$\int_{A_0} P(A|S(x))dP_\theta(x) = P_\theta(A \cap A_0)$$

and for $Q_0 = \sum_i c_i P_{\theta_i}$

$$\int_{A_0} P(A|S(x))dQ_0(x) = Q_0(A \cap A_0) \,.$$

Let

$$g(S(x), \theta) = \frac{dP_\theta}{dQ_0}(x)$$

be the Radon-Nikodym derivative for $(\mathcal{A}(S(X)), Q_0)$. To show that $g(S(x), \theta)$ is the Radon-Nikodym derivative for $(\mathcal{A}, Q_0)$. Setting $A = \Omega$ we have

$$P_\theta(A) = \int_\Omega P(A|S(x))dP_\theta(x) = \int_\Omega E_{Q_0}(I_A(X)|S(x))dP_\theta(x)$$

$$= \int_\Omega E_{Q_0}(I_A(X)|S(x))g(S(x),\theta)dQ_0(x) = \int_\Omega E_{Q_0}(g(S(x),\theta)I_A(X)|S(x))dQ_0(x)$$

$$= \int_\Omega g(S(x),\theta)I_A(x)dQ_0(x) = \int_A g(S(x),\theta)dQ_0(x) \ .$$

So

$$\frac{dP_\theta}{dQ_0}(x) = g(S(x),\theta) \text{ on } \mathcal{A} \ .$$

Conversely, suppose

$$\frac{dP_\theta}{dQ_0}(\mathbf{x}) = g(\mathbf{S}(\mathbf{x}),\theta)$$

to show $P_{Q_0}(A|S(x))$ is a conditional probability function for all $P_\theta \in \mathcal{P}$. Let $g(S(x),\theta) = \frac{dP_\theta}{dQ_0}(x)$ on $\mathcal{A}$. For fixed A and θ define

$$\nu(A) = \int_A dP_\theta(x) \ .$$

Then on $\mathcal{A}(S(X))$ we have

$$\frac{d\nu}{dP_\theta}(x) = E_\theta(I_A(X)|S(x))$$

and

$$\frac{d\nu}{dQ_0}(x) = E_\theta(I_A(X)|S(x))\frac{dP_\theta}{dQ_0}(x) = P_\theta(A|S(x))g(S(x),\theta) \ .$$

Next, on $\mathcal{A}$

$$\frac{d\nu}{dQ_0}(x) = \frac{d\nu}{dP_\theta}(x)\frac{dP_\theta}{dQ_0}(x) = I_A(x)g(S(x),\theta)$$

and

$$\frac{d\nu}{dQ_0}(x) = E_{Q_0}(I_A(X)g(S(X),\theta)|S(x)) = P_{Q_0}(A|S(x))g(S(x),\theta)$$

on $\mathcal{A}(S(X))$. Thus

$$P_{Q_0}(A|S(x))g(S(x),\theta) = P_\theta(A|S(x))g(S(x),\theta)$$

and since $g(S(x),\theta) \neq 0$ a.e. $\mathcal{A}(S(X)), P_\theta)$ we have

$$P_{Q_0}(A|S(x)) = P_\theta(A|S(x))$$

a.e. $(\mathcal{A}(S(X)), P_\theta)$ and $P_{Q_0}(A|S(x))$ is a determination of the conditional probability that does not depend on θ so we have $S(X)$ is sufficient.
To finish the theorem we must show

$$\frac{dP_\theta}{d\mu}(x) = g(S(x),\theta)h(x)$$

if and only if

$$\frac{dP_\theta}{dQ_0}(x) = g(S(x),\theta)$$

for some $h(x)$.
If $Q_0 = \sum_i c_i P_{\theta_i}$ satisfy $P_\theta(A) = 0$ for all θ if and only if $Q_0(A) = 0$ then

$$\frac{dP_\theta}{d\mu}(x) = g(S(x),\theta)h(x)$$

with

$$h(x) = \frac{dQ_0}{d\mu}(x) \ .$$

Converseley, if

$$\frac{dP_\theta}{d\mu}(x) = g(S(x),\theta)h(x)$$

then

$$\frac{dQ_0}{d\mu}(x) = \sum_i c_i g(S(x),\theta_i)h(x) = K(S(x))h(x)$$

and

$$\frac{dP_\theta}{dQ_0}(x) = g^*(S(x),\theta)$$

where $g^*(S(x),\theta) = g(S(x),\theta)/K(S(x))$ when $K(S(x)) > 0$ and 0 otherwise.
∎

Theorem 11.2 *A 1-1 function of a sufficient statistic is also sufficient.*

Proof.
Let $\mathbf{U}(\mathbf{x}) = \mathbf{t}(\mathbf{S}(\mathbf{X}))$ where $\mathbf{t}$ is a 1-1 function. Then by the factorization theorem, the joint density is

$$g(\mathbf{S}(\mathbf{x}), \theta)h(\mathbf{x}) = g(\mathbf{t^{-1}}(\mathbf{U}(\mathbf{x})), \theta)h(\mathbf{x})$$

where $\mathbf{t^{-1}}$ is the inverse function. Thus $\mathbf{U}(\mathbf{X})$ is sufficient.$\blacksquare$

As an example, let $X_1, X_2, \ldots, X_n$ be independent $\mathcal{N}(\mu, \sigma^2)$. Then $(\sum_{i=1}^n X_i, \sum_{i=1}^n X_i^2)$ is sufficient for $\theta = (\mu, \sigma^2) \in (-\infty, \infty) \otimes (0, \infty)$ since

$$f_{X_1,X_2,\ldots,X_n}(x_1, x_2, \ldots, x_n) = \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} e^{-(x_i-\mu)^2/(2\sigma^2)}$$

$$= \frac{e^{-n\mu^2/(2\sigma^2)}}{(\sigma^2 2\pi)^{n/2}} \exp\{-\sum_{i=1}^n x_i^2/(2\sigma^2) + \sum_{i=1}^n x_i(\mu/\sigma^2)\} .$$

Theorem 11.3 *If* $\mathbf{S}(\mathbf{X})$ *is sufficient for* θ *and* φ *is a 1-1 function of* θ *then* $\mathbf{S}(\mathbf{X})$ *is sufficient for* $\eta = \varphi(\theta)$

Proof.
Using the factorization theorem,

$$g(\mathbf{S}(\mathbf{x}), \theta)h(\mathbf{x}) = g(\mathbf{S}(\mathbf{x}), \varphi^{-1}(\eta))h(\mathbf{x})$$

where φ^{-1} is the inverse function.$\blacksquare$

Applying these theorems, if $X_1, X_2, \ldots, X_n$ are independent $\mathcal{N}(\mu, \sigma^2)$, then

$$\bar{X} = \frac{\sum_{i=1}^n X_i}{n}, \quad S = \left(\frac{\sum_{i=1}^n (X_i - \bar{X})^2}{n-1}\right)^{1/2}$$

is sufficient for (μ, σ) since

$$S = \left(\frac{(\sum_{i=1}^n X_i^2) - (\sum_{i=1}^n X_i)^2/n}{n-1}\right)^{1/2}$$

and $(\bar{X}, S)$ is a 1-1 function of $(\sum_{i=1}^n X_i, \sum_{i=1}^n X_i^2)$ and (μ, σ) is a 1-1 function of (μ, σ^2) since $\sigma > 0$.

11.2 Completeness

We say a distribution of a statistic $\mathbf{S}$ is *complete* if the equation

$$E_\theta(h(\mathbf{S})) = 0 \text{ for all } \theta \in \Theta$$

only has the solution $h(\mathbf{s}) = 0$ for almost all[3] $\mathbf{s}$.

For example if X:binomial(n, p) for $0 < p < 1$ then it is complete. Consider

$$\sum_{x=0}^{n} h(x) \begin{pmatrix} n \\ x \end{pmatrix} p^x (1-p)^{n-x} = 0 \text{ for all } p \in (0,1).$$

This is an nth degree polynomial in $p/(1-p)$ that vanishes for more than n values of $p/(1-p)$-in fact for a continuoum of values. Thus the coefficients must all be zero, namely

$$h(x) \begin{pmatrix} n \\ x \end{pmatrix} = 0 \text{ for } x = 0, 1, 2, \ldots, n.$$

Since $\begin{pmatrix} n \\ x \end{pmatrix} \neq 0$ we have $h(x) = 0$ for $x = 0, 1, 2, \ldots, n$ and completeness holds.

For another example, let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ be independent with a uniform$(0, \theta)$ density

$$f_{X_i}(x_i) = \frac{1}{\theta} \text{ for } 0 < x_i < \theta, \;\; 0 < \theta < \infty \; .$$

Then the distribution of $S(\mathbf{X}) = \max\{X_1, X_2, \ldots, X_m\}$ is complete.

$$P(S \leq s) = \prod_{i=1}^{n} P(X_i \leq s) = \left(\frac{s}{\theta}\right)^n I[0 \leq s \leq \theta]$$

and

$$f_S(s) = \frac{ns^{n-1}}{\theta^n} I[0 \leq s \leq \theta] \; .$$

The equation for completeness is

$$\int_0^\theta h(s) \frac{ns^{n-1}}{\theta^n} ds = 0 \text{ for all } \theta \in (0, \infty) \; .$$

[3]It holds for every $\mathbf{s}$ except possibly for $\mathbf{s} \in N$ where $P_\theta(N) = 0$ for all $\theta \in \Theta$.

Multipling by θ^n/n gives

$$\int_0^\theta h(s)s^n ds = 0$$

and differentiating with respect to θ gives

$$h(\theta)\theta^n = 0 \text{ for all } \theta \in (0, \infty).$$

Thus $h(s) = 0$ for all $s \in (0, \infty)$ and completeness holds.

11.3 Exponential Families

We say a family $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ belongs to a k parameter exponential family if the density with respect to μ (e.g. counting or Lebesgue measure) is of the form

$$f_{\mathbf{X}}(\mathbf{x}) = C(\theta) \exp\{\sum_{i=1}^k T_i(\mathbf{x})\eta_i(\theta)\}h(\mathbf{x})$$

where $\mathbf{x} = (x_1, x_2, \ldots, x_n)$, $\theta = (\theta_1, \theta_2, \ldots, \theta_k)$. We assume that neither the T_i nor the η_i satisfy a linear constraint.

As an example, if $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ are independent $\mathcal{N}(\mu, \sigma^2)$ then

$$f_{\mathbf{X}}(\mathbf{x}) = \prod_{i=1}^n \frac{1}{\sigma\sqrt{2\pi}} e^{-(x_i-\mu)^2/(2\sigma^2)}$$

$$= \frac{e^{-n\mu^2/(2\sigma^2)}}{(\sigma^2 2\pi)^{n/2}} \exp\{-\sum_{i=1}^n x_i^2/(2\sigma^2) + \sum_{i=1}^n x_i(\mu/\sigma^2)\}$$

which is a 2 parameter exponential family.

If $\mathbf{X} = (X_1, X_2, \ldots, X_{s-1})$ is multinomial$(n, p_1, p_2, \ldots, p_s)$ then

$$f_{\mathbf{X}}(\mathbf{x}) = \frac{n!}{x_1! x_2! \cdots x_s!} p_1^{x_1} p_2^{x_2} \cdots p_s^{x_s}$$

where $\sum_{i=1}^s p_i = 1$, and $x_s = n - \sum_{i=1}^{s-1} x_i$, with $0 \le x_i \le n$. We can write

$$f_{\mathbf{X}}(\mathbf{x}) = \exp\{n \log_e(p_s)\} \exp\{\sum_{i=1}^{s-1} x_i \log_e(p_i/p_s)\} \frac{n!}{x_1! x_2! \cdots x_s!}$$

which is an $s-1$ parameter exponential family.

Another form of the exponential family uses the natural parameters $\eta = (\eta_1, \eta_2, \ldots, \eta_k)$

$$f_{\mathbf{X}}(\mathbf{x}) = C^*(\boldsymbol{\eta}) \exp\{\sum_{i=1}^{k} T_i(\mathbf{x})\eta_i\} h(\mathbf{x}) \ .$$

The natural parameter space is

$$\boldsymbol{\Lambda} = \{\boldsymbol{\eta} : \int_{-\infty}^{\infty} \exp\{\sum_{i=1}^{k} T_i(\mathbf{x})\eta_i\} h(\mathbf{x}) d\mu(\mathbf{x}) < \infty\} \ .$$

We have the following theorem:

Theorem 11.4 *Let* $\mathbf{X}$ *have density*

$$f_{\mathbf{X}}(\mathbf{x}) = C^*(\eta) \exp\{\sum_{i=1}^{k} T_i(\mathbf{x})\eta_i\} h(\mathbf{x})$$

for $\eta \in \boldsymbol{\Lambda}$*, the natural parameter space. The sufficient statistic* $\mathbf{T} = (T_1, T_2, \ldots, T_k) i^T$ *is complete provided the natural parameter space contains a* k*-dimensional rectangle.*

Proof. See also Lehmann[4].
Without loss of generality, assume the rectangle contains the origin (since we can make a linear translation and absorb the correction into $h(\mathbf{x})$. Consider the equation

$$E_\eta(g(\mathbf{T})) = \int (g^+(\mathbf{T}(\mathbf{x})) - g^-(\mathbf{T}(\mathbf{x})) f_{\mathbf{T}}(\mathbf{T}(\mathbf{x})) d\mu(\mathbf{x}) = 0$$

for all $\eta \in \Lambda$ where $g^+ = \max\{0, g\}$ and $g^- = \max\{0, -g\}$. Then

$$\int \exp\{\sum_{i=1}^{k} T_i(\mathbf{x})\eta_i\} h(\mathbf{x}) g^+(\mathbf{T}(\mathbf{x})) d\mu(\mathbf{x}) = \int \exp\{\sum_{i=1}^{k} T_i(\mathbf{x})\eta_i\} h(\mathbf{x}) g^-(\mathbf{T}(\mathbf{x})) d\mu(\mathbf{x}) \tag{11.1}$$

and for $\boldsymbol{\eta} = \mathbf{0}$

$$\int h(\mathbf{x}) g^+(\mathbf{T}(\mathbf{x})) d\mu(\mathbf{x}) = \int h(\mathbf{x}) g^-(\mathbf{T}(\mathbf{x})) d\mu(\mathbf{x}) \ . \tag{11.2}$$

[4]E.L. Lehmann, *Testing Statistical Hypotheses, Second Edition.* Wadsworth & Brooks/Cole 1991 pages 132-133.

If we divide equation (11.1) by the common value of equation (11.2) we get

$$\int \exp\{\sum_{i=1}^{k} T_i(\mathbf{x})\eta_i\} dP^+(\mathbf{T}(\mathbf{x})) = \int \exp\{\sum_{i=1}^{k} T_i(\mathbf{x})\eta_i\} dP^-(\mathbf{T}(\mathbf{x}))$$

where

$$P^+(\mathbf{T}(\mathbf{x}) \in A) = \int_{\mathbf{T}(\mathbf{x})\in A} h(\mathbf{x})g^+(\mathbf{T}(\mathbf{x}))d\mu(\mathbf{x}) / \int h(\mathbf{y})g^+(\mathbf{T}(\mathbf{y}))d\mu(\mathbf{y}),$$

$$P^-(\mathbf{T}(\mathbf{x}) \in A) = \int_{\mathbf{T}(\mathbf{x})\in A} h(\mathbf{x})g^-(\mathbf{T}(\mathbf{x}))d\mu(\mathbf{x}) / \int h(\mathbf{y})g^-(\mathbf{T}(\mathbf{y}))d\mu(\mathbf{y}) \ .$$

Thus the moment generating funcion for P^+ equals that for P^- for η in a k dimensional interval that contains $\mathbf{0}$. Hence by theorem 8.5, the characteristic functions are equal. By uniqueness of multivariate characteristic functions, (theorem 8.4), $P^+ = P^-$ and so $g^+ = g^-$ and $g = 0$ proving completeness.∎

11.4 Minimum Variance Unbiased Estimation

For point estimation the problem is that of finding a statistic that is close in some sense to a function $\tau(\theta)$ of the unknown parameter θ. In genereal, there is no uniformly best estimator, since, for example, the estimator that is constantly equal 7 is a great estimator if $\tau(\theta) = 7$ but not so good otherwise. One approach is to find estimators $T(\mathbf{X})$ that are *unbiased* for $\tau(\theta)$ in that

$$E_\theta(T(X)) = \int T(\mathbf{x}) f_{\mathbf{X}}(\mathbf{x}|\theta) d\mu(\mathbf{x}) = \tau(\theta) \text{ for all } \theta \in \Theta \ .$$

Then among such estimators, find one that minimizes

$$E_\theta(T(\mathbf{X}) - \tau(\theta))^2 = Var_\theta(T(\mathbf{X}))$$

if such exists.

In many cases, there exists a complete sufficient statistic $S(\mathbf{X})$ and a function of it that is unbiased and it will prove to be a uniformly minimum variance unbiased estimator.

Theorem 11.5 Blackwell-Rao Theorem. *Let* $\mathbf{X}$ *have distribution* $P_\theta \in \mathcal{P} = \{P_\theta : \theta \in \Theta\}$ *with sufficient statistic* $S(\mathbf{X})$ *and let* $T(\mathbf{X})$ *be an unbiased estimator for* $\tau(\theta)$*. If* $E(T(\mathbf{X}) - \tau(\theta))^2 < \infty$ *and if*

$$U(S(\mathbf{X})) = E(T(\mathbf{X})|S(\mathbf{X}))$$

then $U(S(\mathbf{X}))$ *is an unbiased estimator for* $\tau(\theta)$ *and*

$$E(U(S(\mathbf{X})) - \tau(\theta))^2 \leq E(T(\mathbf{X}) - \tau(\theta))^2; .$$

Proof.
By Jensen's inequality, with $E(X) = E(T(\mathbf{X})|S(\mathbf{X}))$, $X = T(\mathbf{X})$, since $h(x) = (x - \theta)^2$ is convex, we have

$$(E(T(\mathbf{X})|S(\mathbf{X})) - \tau(\theta))^2 \leq E((T(\mathbf{X})) - \tau(\theta))^2|S(\mathbf{X}))$$

and taking expectations using $E(E((T(\mathbf{X}) - \tau(\theta))^2|S(\mathbf{X}))) =$
$E(T(\mathbf{X}) - \tau(\theta))^2$

$$E(U(S(\mathbf{X})) - \tau(\theta))^2 \leq E(T(\mathbf{X})) - \tau(\theta))^2 . \blacksquare$$

Thus for minimizing variance among unbiased estimators, we can restrict attention to unbiased functions of the sufficient statistic.

Theorem 11.6 *Let* $\mathbf{X}$ *have distribution* $P_\theta \in \mathcal{P} = \{P_\theta : \theta \in \Theta\}$ *with sufficient statistic* $\mathbf{S}(\mathbf{X})$ *that is complete. Then if* $U(\mathbf{S}(\mathbf{X}))$ *is unbiased for* $\tau(\theta)$*, it is the uniformly minimum variance unbiased (U.M.V.U.) estimator for* $\tau(\theta)$*.*

Proof.
By the Blackwell-Rao theorem let $U_1(\mathbf{S}(\mathbf{X}))$ and $U_2(\mathbf{S}(\mathbf{X}))$ be unbiased for $\tau(\theta)$. Then for all $\theta \in \Theta$

$$E_\theta(U_1(S(\mathbf{X})) - U_2(\mathbf{S}(\mathbf{X})) = \tau(\theta) - \tau(\theta) = 0$$

and $g(\mathbf{S}(\mathbf{X})) = U_1\mathbf{S}(\mathbf{X})) - U_2(\mathbf{S}(\mathbf{X})) = 0$ a.e. Thus

$$U_1(\mathbf{S}(\mathbf{X})) = U_2(\mathbf{S}(\mathbf{X})) \text{ a.e. } \mathcal{P}$$

and there is only one such unbiased estimator that is a function of $\mathbf{S}(\mathbf{X})$ (up to sets of P_θ measure zero. $\blacksquare$

Thus if there is a complete sufficient statistic, to obtain the U.M.V.U. estimator we look for a function of $\mathbf{S}(\mathbf{X})$ that is unbiased for $\tau(\theta)$.

There are basically two ways to find such a function.

1. Find any unbiased estimator $T(\mathbf{X})$. Then calculate $U(\mathbf{S}(\mathbf{X})) = E(T(\mathbf{X})|\mathbf{S}(\mathbf{X}))$ which is unique by completeness.

2. Solve the functional equation for $U(\mathbf{s})$

$$E_\theta(U(\mathbf{S})) = \int U(\mathbf{s}) f_{\mathbf{S}}(\mathbf{s}) d\mu(\mathbf{s}) = \tau(\theta) \text{ for all } \theta \in \Theta \ .$$

For an example, let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ where X_i are independent $\mathcal{N}(\mu, \sigma^2)$. Let $\theta = (\mu, \sigma^2)$. To find the U.M.V.U. estimator for (a) $\tau(\theta) = \mu$ and (b) $\tau(\theta) = \sigma^2$. By exponential family theory, $\mathbf{S}(\mathbf{X}) = (\sum_{i=1}^n X_i, \sum_{i=1}^n X_i^2)$ is sufficient and complete since the natural parameter space contains a 2 dimensional rectangle.
(a) Using the second method above we have

$$E_\theta(\sum_{i=1}^n X_i) = n\mu, \text{ so } E_\theta \bar{X} = \tau(\theta) = \mu$$

and $\bar{X} = \sum_{i=1}^n X_i/n$ is a function of $\mathbf{S}(\mathbf{X})$ that is unbiased and hence U.M.V.U. for estimating μ.
(b) We have

$$E_\theta(S^2) = E_\theta(\frac{\sigma^2}{(n-1)}\chi^2_{(n-1)}) = \frac{\sigma^2}{(n-1)}(n-1) = \tau(\theta) = \sigma^2$$

and $S^2 = [\sum_{i=1}^n X_i^2 - (\sum_{i=1}^n X_i)^2/n]/(n-1)$ is a function of $\mathbf{S}(\mathbf{X})$ that is unbiased and U.M.V.U. for estimating σ^2.

For another example, let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ where X_i are independent with discrete density

$$P_M(X_i = k) = \frac{1}{2M+1} \text{ for } k \text{ an integer, } -M \le k \le M$$

where $\theta = M$ is an unknown integer parameter $M \in \{0, 1, 2, \ldots, \infty\}$. To derive the U.M.V.U. estimator for $\tau(\theta) = M$.

$$P(\mathbf{X} = (x_1, x_2, \ldots, x_n)) = \frac{1}{(2M+1)^n} I_{[\max_{i=1}^n\{|x_i|\} \le M]}(\mathbf{x}) I_{[0 \le \min_{i=1}^n\{|x_i|\}]}(\mathbf{x})$$

so by the Neyman-Fisher factorization theorem $\mathbf{S}(\mathbf{X}) = \max_{i=1}^n\{|X_i|\}$ is sufficient for M.

$$P(\max_{i=1}^n\{|X_i|\} \le s) = \left(\frac{2s+1}{2M+1}\right)^n \text{ for } s = 0, 1, 2, \ldots, M$$

and

$$P(\max_{i=1}^{n}\{|X_i|\} = 0) = \left(\frac{1}{2M+1}\right)^n$$

$$P(\max_{i=1}^{n}\{|X_i|\} = s) = \left(\frac{2s+1}{2M+1}\right)^n - \left(\frac{2(s-1)+1}{2M+1}\right)^n \text{ for } s = 1, 2, \ldots, M \ .$$

To show completeness

$$E_M(h(S)) = 0 \text{ for all } M \in \{0, 1, 2, \ldots, \infty\}$$

For $M = 0$ this gives

$$h(0) \times 1 = 0 \text{ and } h(0) = 0 \ .$$

Using induction, assume $h(s) = 0$ for $s = 1, 2, \ldots, N-1$, to show $h(N) = 0$. Let $M = N$ then the equation for completeness gives

$$h(0)P(S=0)+h(1)P(S=1)+\cdots+h(N-1)P(S=N-1)+h(N)P(S=N) = 0$$

and using the induction hypothesis

$$h(N)P(S = N) = 0 \text{ and } h(N) = 0 \ .$$

Thus by induction $h(s) = 0$ for $s = 0, 1, 2, \ldots, \infty$ and completeness is proved. Using the first method, we find a simple unbiased estimator based on $|X_1|$

$$E_M(T(|X_1|)) = M \text{ for all } M = 0, 1, 2, \ldots, \infty$$

Now first, playing around, we find an estimator $R(|X_1|)$ that is linear in M

$$R(k) = \begin{cases} 1 & \text{for } k = 0 \\ 4k & \text{for } k = 1, 2, \ldots, M. \end{cases}$$

$$E(R(|X_1|) = 1\frac{1}{2M+1} + \sum_{k=1}^{M} 4k\frac{2}{2M+1} = \frac{1+4M(M+1)}{2M+1} = 2M+1$$

so

$$T(|X_1|) = \frac{(R(|X_1|)-1)}{2} = \begin{cases} 0 & \text{for } |X_1| = 0 \\ 2|X_1| - 1/2 & \text{for } |X_1| > 0 \end{cases}$$

is unbiased for M. We now compute the U.M.V.U estimator

$$U(s) = E(T(|X_1|)|S = s) \ .$$

The conditional distribution is

$$P(|X_1| = k|S = s) = \frac{P(|X_1| = k, S = s)}{P(S = s)}$$

$$= \begin{cases} P(|X_1| = 0, \max_{i=2}^n\{|X_i|\} = 0)/P(S = 0) & \text{for } k = s = 0 \\ P(|X_1| = 0, \max_{i=2}^n\{|X_i|\} = s)/P(S = s) & \text{for } 0 = k < s \\ P(|X_1| = k, \max_{i=2}^n\{|X_i|\} = s)/P(S = s) & \text{for } 1 \le k < s \\ P(|X_1| = s, \max_{i=2}^n\{|X_i|\} \le s)/P(S = s) & \text{for } 1 \le k = s\ . \end{cases}$$

and after canceling $(2M + 1)^n$ from numerator and denominator

$$= \begin{cases} 1 & \text{for } k = s = 0 \\ \frac{\left\{(2s+1)^{n-1} - (2(s-1)+1)^{n-1}\right\}}{\{(2s+1)^n - (2(s-1)+1)^n\}} & \text{for } 0 = k < s \\ 2\frac{\left\{(2s+1)^{n-1} - (2(s-1)+1)^{n-1}\right\}}{\{(2s+1)^{n-1} - (2(s-1)+1)^{n-1}\}} & \text{for } 1 \le k < s \\ 2\frac{(2s+1)^{n-1}}{\{(2s+1)^{n-1} - (2(s-1)+1)^{n-1}\}} & \text{for } 1 \le k = s \end{cases}$$

Then for $s > 0$

$$U(s) = \sum_{k=1}^{s} 2kP(|X_1| = k|S = s)) =$$

$$\sum_{k=1}^{s-1} \frac{(2k - 1/2)2\{(2s + 1)^{n-1} - (2(s - 1) + 1)^{n-1}\}}{(2s + 1)^n - (2(s - 1) + 1)^n} + \frac{(2s - 1/2)2(2s + 1)^{n-1}}{(2s + 1)^n - (2(s - 1) + 1)^n}$$

$$= \frac{(2s(s - 1) - (s - 1))\{(2s + 1)^{n-1} - (2(s - 1) + 1)^{n-1}\} + (4s - 1)(2s + 1)^{n-1}}{(2s + 1)^n - (2(s - 1) + 1)^n}$$

$$= \frac{s(2s + 1)^n - (s - 1)(2(s - 1) + 1)^n}{(2s + 1)^n - (2(s - 1) + 1)^n} \text{ for } s = 1, 2, \ldots, M$$

and for $s = 0$,

$$U(0) = E(T(|X_1|)|S = 0) = 0 \times 1 = 0\ .$$

As a check, canceling $(2s+1)^n - (2(s-1)+1)^n$ from numerator and denominator

$$E_M(U(S)) = 0 + \sum_{s=1}^{M} \frac{s(2s + 1)^n - (s - 1)(2(s - 1) + 1)^n}{(2M + 1)^n} = \frac{M(2M + 1)^n}{(2M + 1)^n} = M$$

from the telescoping sum. It is the unbiased estimator for M based on the complete sufficients statistic S and is U.M.V.U.

For another example, let $Y_1, Y_2, \ldots, Y_n$ be independent normal with

$$E_\theta(Y_i) = \sum_{j=1}^{p} x_{ij}\beta_j \text{ and } Var_\theta(Y_i) = \sigma^2 \tag{11.3}$$

where $\theta = (\beta_1, \beta_2, \ldots, \beta_p, \sigma^2)$.

First, let $\tau(\theta) = \psi = \sum_{j=1}^{p} a_j\beta_j$ for given $\mathbf{a}^T = (a_1, a_2, \ldots, a_p)$. The joint distribution is

$$\left(\frac{1}{\sigma^2 2\pi}\right)^{n/2} \exp\{-\sum_{i=1}^{n}(Y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2/(2\sigma^2)\}$$

$$= C(\theta)\exp\{-\sum_{i=1}^{n} Y_i^2/(2\sigma^2) + \sum_{j=1}^{p}(\beta_j/\sigma^2)\sum_{i=1}^{n} Y_i x_{ij}\}$$

where $C(\theta)$ is a constant. Thus

$$\sum_{i=1}^{n} Y_i^2, \text{ and } \sum_{i=1}^{n} Y_i x_{ij} \text{ for } j = 1, 2, \ldots, p$$

is sufficient for θ. It is complete by exponential family theory since the parameter space contains a $k = p + 1$ dimensional rectangle provided

$$\mathbf{X}^{n\times p} = \begin{pmatrix} x_{11} & x_{12} & \ldots & x_{1p} \\ x_{21} & x_{22} & \ldots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \ldots & x_{np} \end{pmatrix}$$

is of rank p. Then if $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_n)^T$ and $\beta = (\beta_1, \beta_2, \ldots, \beta_p)^T$, we have $\mathbf{Y}$ has a $\mathcal{N}_n(\mathbf{X}\beta, \sigma^2\mathbf{I}_n)$ distribution where $\mathbf{I}_n$ is the $n \times n$ identity matrix and

$$\mathbf{Y}^T\mathbf{Y} \text{ and } \mathbf{X}^T\mathbf{Y}$$

are the sufficient statistics. Using

$$E(\mathbf{X}^T\mathbf{Y}) = \mathbf{X}^T\mathbf{X}\beta,$$

the U.M.V.U. estimator for $\psi = \mathbf{a}^T\beta$ is

$$\hat{\psi} = \mathbf{a}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y} \ .$$

If we form the **QR** decomposition for **X** (see for example Golub and Van Loan[5] (1989) pages 211-233)

$$\mathbf{X}^{n\times p} = \mathbf{Q}^{n\times n}\mathbf{R}^{n\times p}$$

where **Q** is orthogonal, ($\mathbf{Q}^T\mathbf{Q} = \mathbf{I}_n = \mathbf{Q}\mathbf{Q}^T$), and

$$\mathbf{R}^{n\times p} = \begin{pmatrix} r_{11} & r_{12} & r_{13} & \dots & r_{1p} \\ 0 & r_{22} & r_{23} & \dots & r_{2p} \\ 0 & 0 & r_{33} & \dots & r_{3p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & r_{pp} \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{R}_{11}^{p\times p} \\ \mathbf{0} \end{pmatrix}$$

and $\mathbf{R}_{11}$ is upper triangular of rank p. If we partition $\mathbf{Q}^T$

$$\mathbf{Q}^T = \begin{pmatrix} \mathbf{Q}_1^T \\ \mathbf{Q}_2^T \end{pmatrix}$$

where $\mathbf{Q}_1^T$ is of dimension $p \times n$ then we can solve for $\hat{\beta}$ in the equation

$$\mathbf{R}_{11}\hat{\beta} = \mathbf{Z} \text{ where } \mathbf{Z} = \mathbf{Q}_1^T\mathbf{Y}$$

and then calculate the estimate $\hat{\psi} = \mathbf{a}^T\hat{\beta}$.

Next, let $\tau(\theta) = \sigma^2$ and consider

$$(\mathbf{Y} - \mathbf{X}\hat{\beta})^T(\mathbf{Y} - \mathbf{X}\hat{\beta}) = \mathbf{Y}^T\mathbf{Y} - \hat{\beta}^T\mathbf{X}^T\mathbf{X}\hat{\beta}$$

which is a function of the sufficient statistic. Substituting **QR** for **X** gives

$$\mathbf{Y}^T\mathbf{Q}\left(\mathbf{I}_n - \begin{pmatrix} \mathbf{I}_p & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\right)\mathbf{Q}^T\mathbf{Y} = \mathbf{Y}^T\mathbf{Q}\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{(n-p)} \end{pmatrix}\mathbf{Q}^T\mathbf{Y} \ .$$

[5]Golub, G.H. and C.F. Van Loan, 1989, *Matrix Computations, Second Edition.* Johns Hopkins University Press, Baltimore.

From

$$E(\mathbf{Q}^T\mathbf{Y}) = \mathbf{Q}^T\mathbf{Q}\mathbf{R} = \mathbf{R} = \begin{pmatrix} \mathbf{R}_{11}^{p\times p} \\ \mathbf{0} \end{pmatrix}$$

we have

$$\mathbf{Y}^T\mathbf{Q}\begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{(n-p)} \end{pmatrix}\mathbf{Q}^T\mathbf{Y} = \mathbf{W}^T\mathbf{W} = \sigma^2\chi^2_{(n-p)}(0)$$

where $\mathbf{W} = \mathbf{Q}_2^T\mathbf{Y}$ has a $\mathcal{N}_{(n-p)}(\mathbf{0}, \sigma^2\mathbf{I}_{(n-p)})$ distribution. Since $\sigma^2\chi^2_{(n-p)}(0)$ has expectation $\sigma^2(n-p)$,

$$S^2 = \frac{(\mathbf{Y} - \mathbf{X}\hat{\beta})^T(\mathbf{Y} - \mathbf{X}\hat{\beta})}{(n-p)} = \frac{\mathbf{W}^T\mathbf{W}}{(n-p)}$$

is the U.M.V.U. estimator for σ^2.

For

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Y}$$

the variance covariance matrix is

$$\sigma^2(\mathbf{X}^T\mathbf{X})^{-1} = \sigma^2\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T}$$

which is estimated by

$$S^2(\mathbf{X}^T\mathbf{X})^{-1} = S^2\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T} \ .$$

To calculate these estimators, we can obtain the **QR** decomposition by Householder transformations and then

$$\begin{pmatrix} \mathbf{Z} \\ \mathbf{W} \end{pmatrix} = \mathbf{Q}^T\mathbf{Y} \ .$$

The C++ code **Regress.cpp** in **Appendix C** can be compiled to produce an executable program. For example, using the gnu C++ compiler under LINUX, we compile it as follows:

% g++ -o Regress Regress.cpp

We then execute it using the data file named *data1* as follows:

% Regress data1

If the input file *Regress.data* is:
4 2
2 1
4 1 2
5 1 3
9 1 5
8 1 4
Then the program output is:

```
(n,p)=(4,2)

(a[1],a[2])=(2,1)

Y[i]   : X[i,j] i=1,2,...,n, j=1,2,...,p
----------------------------------------
4      : 1 2
5      : 1 3
9      : 1 5
8      : 1 4

b=( 0.200000, 1.800000 )'

Cov(b) estimate
  1.080000  -0.280000
 -0.280000   0.800000

a'b= 2.200000

Estimate of Var(a'b)=3.280000

S^2= (Y-Xb)'(Y-Xb)/(n-p)= 0.400000
```

For the important special case of simple linear regression

$$Y_i = \beta_0 + x_i\beta_1 + \varepsilon_i$$

where ε_i are independent $\mathcal{N}(0, \sigma^2)$ for $i = 1, 2, \ldots, n$, we have closed form expressions for the U.M.V.U. estimators. In particular,

$$\hat{\beta}_1(n) = \frac{S_{xY}(n)}{S_x^2(n)}, \quad \hat{\beta}_0(n) = \bar{Y}_n - \hat{\beta}_1(n)\bar{x}_n$$

and

$$\hat{\sigma}^2 = \frac{S_e^2(n)}{(n-2)}$$

where

$$S_{xY}(n) = \sum_{i=1}^{n}(x_i - \bar{x}_n)(Y_i - \bar{Y}_n), \quad S_X^2(n) = \sum_{i=1}^{n}(x_i - \bar{x})^2$$

$$S_e^2(n) = \sum_{i=1}^{n}(Y_i - \bar{Y}_n - \hat{\beta}_1(n)(x_i - \bar{x}_n))^2 \ .$$

and

$$\bar{x}_n = \frac{\sum_{i=1}^{n} x_i}{n}, \quad \bar{Y}_n = \frac{\sum_{i=1}^{n} Y_i}{n} \ .$$

We can calculate these terms by updating using the formulae[6]

$$S_{xY}(n+1) = S_{xY}(n) + \frac{n}{(n+1)}(x_{n+1} - \bar{x}_n)(Y_{n+1} - \bar{Y}_n)$$

$$S_x^2(n+1) = S_x^2(n) + \frac{n}{(n+1)}(x_{n+1} - \bar{x}_n)^2$$

$$S_e^2(n+1) = S_e^2(n) + \frac{n}{(n+1)}(Y_{n+1} - \bar{Y}_n - \hat{\beta}_1(n)(x_{n+1} - \bar{x}_n))^2 \frac{S_x^2(n)}{S_x^2(n+1)}$$

with starting values $S_x^2(1) = 0$, $S_{xY}(1) = 0$, $S_e^2(1) = 0$ and $\bar{x}_1 = x_1$, $\bar{Y}_1 = Y_1$.

We can also remove an incorrect entry using

$$S_e^2(n) = S_e^2(n+1) - \frac{(n+1)}{n}(Y_{n+1} - \bar{Y}_{n+1} - \hat{\beta}_1(n+1)(X_{n+1} - \bar{X}_{n+1}))^2 \frac{S_x^2(n+1)}{S_x^2(n)}$$

where

$$S_x^2(n) = S_x^2(n+1) - \frac{(n+1)}{n}(x_{n+1} - \bar{x}_{n+1})^2 \ .$$

Golub and Styan (1973) [7] give update formulae for general linear regression.

[6] Klotz, J.H.(1995) Updating Simple Linear regression. *Statistica Sinica* **5**, 399-403.

[7] Golub, G.H. and Styan, G.P.H. (1973). Numerical computations for univariate linear models. *Journal of Statistical Computation and Simulation* **2**, 256-274.

11.5 Cramér-Rao-Frechèt Information Lower Bound

Theorem 11.7 *Let* $\mathbf{X}$ *have density* $f(\mathbf{x}|\theta)$ *for* $\theta \in \Theta$ *with respect to a measure* $\mu(\mathbf{x})$ *and assume*
1. *The set* $A = \{\mathbf{x} : f(\mathbf{x}|\theta) > 0\}$ *does not depend on* θ *and for all* $\mathbf{x} \in A$, $\theta \in \Theta$, $(\partial/\partial\theta)\ln(f(\mathbf{x}|\theta))$ *exists and is finite.*
2. *If* $T(\mathbf{X})$ *is a statistic such that* $E_\theta|T(\mathbf{X})| < \infty$ *for all* $\theta \in \Theta$, *then*

$$\frac{\partial}{\partial\theta}\int T(\mathbf{x})f(\mathbf{x}|\theta)d\mu(\mathbf{x}) = \int \frac{\partial}{\partial\theta}T(\mathbf{x})f(\mathbf{x}|\theta)d\mu(\mathbf{x}) \ .$$

3. *The information matrix*

$$\mathcal{I}(\theta) = -E_\theta\left(\frac{\partial^2}{\partial\theta\partial\theta^T}\ln(f(\mathbf{X}|\theta))\right) = E_\theta\left(\frac{\partial}{\partial\theta}\ln(f(\mathbf{X}|\theta))\frac{\partial}{\partial\theta^T}\ln(f(\mathbf{X}|\theta))\right)$$

is positive definite.
Then if $\delta(\mathbf{X})$ *is any estimator with* $E_\theta(\delta^2(\mathbf{X})) < \infty$ *we have*

$$Var_\theta(\delta(\mathbf{X})) \geq \alpha^T\mathcal{I}^{-1}(\theta)\alpha$$

where

$$\alpha = \frac{\partial}{\partial\theta}E_\theta(\delta(\mathbf{X})) \ .$$

We first prove some lemmas.

Lemma 11.2 *For any random variables* $X_1, X_2, \ldots, X_r$ *with finite second moments, the covariance matrix* $C = (Cov(X_i, X_j))$ *is positive semidefinite. It is positive definite if there do not exist constants* $\mathbf{a} = (a_1, a_2, \ldots, a_r)^T$ *and* b *such that* $P(\sum_{i=1}^r a_iX_i = b) = 1$.

Proof of lemma.

$$Var_\theta(\sum_{i=1}^r a_iX_i) = \mathbf{a}^TC\mathbf{a} \geq 0$$

and it is strictly positive if no such constants $\mathbf{a}$ and b exist. ∎

Lemma 11.3 *Let $X_1, X_2, \ldots, X_r, Y$ be random variables with finite second moments and define the multiple correlation coefficient $\rho^* = \sup_{\mathbf{a}} Corr(\sum_{i=1}^r a_i X_i, Y)$. If $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots, \gamma_r)^T$ where $\gamma_i = Cov(X_i, Y)$ and $\boldsymbol{\Sigma} = Cov(X_1, X_2, \ldots, X_r)$ is positive definite, then*

$$(\rho^*)^2 = \boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma} / Var(Y) \ .$$

Proof of lemma.
Since the correlation coefficient is invariant under scale changes, the vector $\mathbf{a}$ that maximizes $Corr(\sum_{i=1}^r a_i X_i, Y)$ is not uniquely defined. Without loss of generality, assume $Var_\theta(\sum_{i=1}^r a_i X_i) = \mathbf{a}^T \boldsymbol{\Sigma} \mathbf{a} = 1$. Then to maximize $\mathbf{a}^T \boldsymbol{\gamma}$ subject to $\mathbf{a}^T \boldsymbol{\Sigma} \mathbf{a} = 1$ using LaGrange multipliers, we can maximize

$$\mathbf{a}^T \boldsymbol{\gamma} - \frac{\lambda}{2} \mathbf{a}^T \boldsymbol{\Sigma} \mathbf{a} \ .$$

Differentiating with respect to $\mathbf{a}$ and setting it equal $\mathbf{0}$ gives

$$\boldsymbol{\gamma} - \lambda \boldsymbol{\Sigma} \mathbf{a} = \mathbf{0}^{r \times 1}$$

or

$$\mathbf{a} = \boldsymbol{\Sigma}^{-1} \lambda^{-1} \boldsymbol{\gamma} \ .$$

Substituting into the side condition $\mathbf{a}^T \boldsymbol{\Sigma} \mathbf{a} = 1$ gives

$$(\boldsymbol{\gamma}^T \lambda^{-1} \boldsymbol{\Sigma}^{-1}) \boldsymbol{\Sigma} (\boldsymbol{\Sigma}^{-1} \lambda^{-1} \boldsymbol{\gamma}) = \lambda^{-2} \boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma} = 1$$

and

$$\lambda = \pm \sqrt{\boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma}} \text{ and } (\mathbf{a}^T \boldsymbol{\gamma})^2 = \left(\frac{\boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma}}{\sqrt{\boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma}}} \right)^2 = \boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma} \ .$$

From this

$$(\rho^*)^2 = Corr^2(\sum_{i=1}^r a_i X_i, Y) = \frac{Cov^2(\sum_{i=1}^r X_i, Y)}{Var(\sum_{i=1}^r a_i X_i) Var(Y)}$$

$$= \frac{(\mathbf{a}^T \boldsymbol{\gamma})^2}{Var(\sum_{i=1}^r a_i X_1) Var(Y)} = \frac{\boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma}}{Var(\sum_{i=1}^r a_i X_i) Var(Y)} = \frac{\boldsymbol{\gamma}^T \boldsymbol{\Sigma}^{-1} \boldsymbol{\gamma}}{Var(Y)}$$

since we set $Var(\sum_{i=1}^r a_i X_i) = 1$.$\blacksquare$
Proof of theorem (11.7).
Replacing Y by $\delta(\mathbf{X})$, X_i by

$$\frac{\partial}{\partial \theta_i} \ln(f(\mathbf{X}|\theta))$$

and γ_i by

$$\alpha_i = Cov(\delta(\mathbf{X}), \frac{\partial}{\partial \theta_i} \ln(f(\mathbf{X}|\theta)))$$

in the lemmas gives the result since

$$\Sigma_{ij} = Cov(\frac{\partial}{\partial \theta_i} \ln(f(\mathbf{X}|\theta), \frac{\partial}{\partial \theta_j} \ln(f(\mathbf{X}|\theta)))) = \mathcal{I}_{ij}(\theta)$$

and

$$1 \geq (\rho^*)^2 = \frac{\boldsymbol{\alpha}^T \mathcal{I}^{-1}(\theta) \boldsymbol{\alpha}}{Var_\theta(\delta(\mathbf{X}))} \,.\blacksquare$$

As an example, let $X_1, X_2, \ldots, X_n$ be independent with density

$$f_{X_i}(x_i|\theta) = \frac{x_i^{\alpha-1} e^{-x_i/\sigma}}{\sigma^\alpha \Gamma(\alpha)} \text{ for } x_i > 0,\ 0 \text{ elsewhere}$$

where $\theta = (\alpha, \sigma)^T$. We calculate for a single observation

$$-E\left(\frac{\partial^2 \ln(f_X(x|\theta))}{\partial\theta\partial\theta^T}\right) = \begin{pmatrix} \psi'(\alpha) & 1/\sigma \\ 1/\sigma & \alpha/\sigma \end{pmatrix} = \mathcal{I}(\theta)$$

where $\psi(\alpha) = d\ln(\Gamma(\alpha))/d\alpha$ is the digamma function. For a sample, the information is $n\mathcal{I}(\theta)$. For estimating $g(\theta) = \sigma$ we have

$$\alpha^T = \left(\frac{\partial g(\theta)}{d\alpha}, \frac{\partial g(\theta)}{d\sigma}\right) = (0, 1)\ .$$

For unbiased estimators $\delta(X_1, X_2, \ldots, X_n)$ of σ we have

$$Var_\theta(\delta(X_1, X_2, \ldots, X_n)) \geq (0,1)(n\mathcal{I}(\theta))^{-1} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{\sigma^2}{n(\alpha - (\psi'(\alpha))^{-1})}\ .$$

Since $\Gamma(\alpha) = \Gamma(1+\alpha)/\alpha$ we have $\psi'(\alpha) = 1/\alpha^2 + \psi'(1+\alpha)$ and

$$0 < \frac{1}{\alpha} = \sum_{k=0}^{\infty} \frac{1}{(\alpha+k)(\alpha+k+1)} < \sum_{k=0}^{\infty} \frac{1}{(\alpha+k)^2} = \psi'(\alpha)\ .$$

The univariate information lower bound for unbiased estimation of σ is

$$Var_\theta(\delta(X_1, X_2, \ldots, X_n)) \geq \frac{\sigma^2}{n\alpha}$$

which is smaller than the above bivariate information lower bound.

Theorem 11.8 *If we have calculated the information $\mathcal{I}(\theta)$ in terms of a parameter $\theta = (\theta_1, \theta_2, \ldots, \theta_K)^T$ and we wish to calculate it for a different parameterization $\eta = (\eta_1, \eta_2, \ldots, \eta_K)^T$ then, provided the derivatives exist,*

$$\mathcal{I}(\eta) = \left(\frac{\partial \theta^T}{\partial \eta}\right) \mathcal{I}(\theta) \left(\frac{\partial \theta}{\partial \eta^T}\right)$$

where

$$\left(\frac{\partial \theta}{\partial \eta^T}\right) = \begin{pmatrix} \partial\theta_1/\partial\eta_1 & \partial\theta_1/\partial\eta_2 & \ldots & \partial\theta_1/\partial\eta_K \\ \partial\theta_2/\partial\eta_1 & \partial\theta_2/\partial\eta_2 & \ldots & \partial\theta_2/\partial\eta_K \\ \vdots & \vdots & \ddots & \vdots \\ \partial\theta_K/\partial\eta_1 & \partial\theta_K/\partial\eta_2 & \ldots & \partial\theta_K/\partial\eta_K \end{pmatrix} = \left(\frac{\partial \eta}{\partial \theta^T}\right)^{-1} = \left(\frac{\partial \theta^T}{\partial \eta}\right)^T .$$

Proof.
By the chain rule,

$$\frac{\partial \mathcal{L}(\eta|\mathbf{x})}{\partial \eta_j} = \sum_{i=1}^{K} \frac{\partial \mathcal{L}(\theta|\mathbf{x})}{\partial \theta_i} \frac{\partial \theta_i}{\partial \eta_j}$$

or in terms of vectors

$$\left(\frac{\partial \mathcal{L}(\eta|\mathbf{x})}{\partial \eta^T}\right)^{1\times K} = \left(\frac{\partial \mathcal{L}(\theta|\mathbf{x})}{\partial \theta^T}\right)^{1\times K} \left(\frac{\partial \theta}{\partial \eta^T}\right)^{K\times K} .$$

Then $\mathcal{I}(\eta) =$

$$E\left(\frac{\partial \mathcal{L}(\eta|\mathbf{X})}{\partial \eta} \frac{\partial \mathcal{L}(\eta|\mathbf{X})}{\partial \eta^T}\right) = E\left(\left(\frac{\partial \theta^T}{\partial \eta}\right)\left(\frac{\partial \mathcal{L}(\theta|\mathbf{X})}{\partial \theta}\right)\left(\frac{\partial \mathcal{L}(\theta|\mathbf{X})}{\partial \theta^T}\right)\left(\frac{\partial \theta}{\partial \eta^T}\right)\right)$$

$$= \left(\frac{\partial \theta^T}{\partial \eta}\right) E\left(\left(\frac{\partial \mathcal{L}(\theta|\mathbf{X})}{\partial \theta}\right)\left(\frac{\partial \mathcal{L}(\theta|\mathbf{X})}{\partial \theta^T}\right)\right)\left(\frac{\partial \theta}{\partial \eta^T}\right) = \left(\frac{\partial \theta^T}{\partial \eta}\right) \mathcal{I}(\theta) \left(\frac{\partial \theta}{\partial \eta^T}\right) .$$

Finally, the $K \times K$ identity matrix

$$I_K = \left(\frac{\partial \eta}{\partial \eta^T}\right) = \left(\frac{\partial \eta}{\partial \theta^T}\right)\left(\frac{\partial \theta}{\partial \eta^T}\right)$$

using the chain rule. Inverting gives

$$\left(\frac{\partial \eta}{\partial \theta^T}\right)^{-1} = \left(\frac{\partial \theta}{\partial \eta^T}\right) . \blacksquare$$

For an example, let $\mathbf{X}_i$ be independent for $i = 1, 2, \ldots, n$ with

$$f_{\mathbf{X_i}}(\mathbf{x_i}|\theta) = p_1^{x_{i1}} p_2^{x_{i2}} \cdots p_K^{x_{ik}}$$

where $x_{ij} \in \{0, 1\}$, $\sum_{j=1}^{K} x_{ij} = 1$ and $\theta = (\ln(p_1/p_K), \ln(p_2/p_K), \ldots, \ln(p_{K-1}/p_K))^T$. The information

$$\mathcal{I}(\theta) = \begin{pmatrix} p_1(1-p_1) & -p_1p_2 & \cdots & -p_1p_{K-1} \\ -p_2p_1 & p_2(1-p_2) & \cdots & -p_2p_{K-1} \\ \vdots & \vdots & \ddots & \vdots \\ -p_{K-1}p_1 & -p_{K-1}p_2 & \cdots & p_{K-1}(1-p_{K-1}) \end{pmatrix} .$$

To calculate the information for the parameter $\eta = (p_1, p_2, \ldots, p_{K-1})^T$ we have

$$\mathcal{I}(\eta) = \left(\frac{\partial \theta^T}{\partial \eta}\right) \mathcal{I}(\theta) \left(\frac{\partial \theta}{\partial \eta^T}\right)$$

$$= \begin{pmatrix} \frac{1}{p_1} + \frac{1}{p_K} & \frac{1}{p_K} & \cdots & \frac{1}{p_K} \\ \frac{1}{p_K} & \frac{1}{p_2} + \frac{1}{p_K} & \cdots & \frac{1}{p_K} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{p_K} & \frac{1}{p_K} & \cdots & \frac{1}{p_{K-1}} + \frac{1}{p_K} \end{pmatrix}$$

and also

$$\mathcal{I}^{-1}(\eta) = \begin{pmatrix} p_1(1-p_1) & -p_1p_2 & \cdots & -p_1p_{K-1} \\ -p_2p_1 & p_2(1-p_2) & \cdots & -p_2p_{K-1} \\ \vdots & \vdots & \ddots & \vdots \\ -p_{K-1}p_1 & -p_{K-1}p_2 & \cdots & p_{K-1}(1-p_{K-1}) \end{pmatrix}$$

since

$$\left(\frac{\partial \theta^T}{\partial \eta}\right) = \begin{pmatrix} \frac{1}{p_1} + \frac{1}{p_K} & \frac{1}{p_K} & \cdots & \frac{1}{p_K} \\ \frac{1}{p_K} & \frac{1}{p_2} + \frac{1}{p_K} & \cdots & \frac{1}{p_K} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{p_K} & \frac{1}{p_K} & \cdots & \frac{1}{p_{K-1}} + \frac{1}{p_K} \end{pmatrix} .$$

11.6 Maximum Likelihood Estimation

Another approach to point estimation involves adjusting the parameters of the joint density (with respect to a dominating measure μ) to make it a maximum at the observed values of the random variables. The joint density, when viewed as a function of the parameters θ for fixed $\mathbf{x}$ is called the likelihood.

$$L(\theta|\mathbf{x}) = f_{\mathbf{X}}(\mathbf{x}|\theta) \text{ for } \theta \in \Theta$$

where $f_{\mathbf{X}}(\mathbf{x}|\theta)$ is the joint density function of $\mathbf{x}$ for fixed θ. The value $\hat{\theta}(\mathbf{X})$ that maximizes $L(\theta|\mathbf{X})$ for $\theta \in \Theta$, if it exists, is called the maximum likelihood estimator.

For example, let X have the binomial(n, p) distribution. Then

$$L(p|x) = p^x(1-p)^{n-x}\begin{pmatrix} n \\ x \end{pmatrix} \text{ for } p \in [0,1] \ .$$

To find the maximum likelihood estimator of p we can differentiate $\log_e(L(p|x))$, set it to zero, and solve for p, since $\log_e(L(p|x))$ is a unimodal differentiable function of p and an increasing function of $L(p|x)$ so that a value of p maximizing $\log_e(L(p|x))$ maximizes $L(p|x)$:

$$\frac{d}{dp}\log_e(L(p|x)) = \frac{d}{dp}\left(x\log_e(p) + (n-x)\log_e(1-p) + \log_e\begin{pmatrix} n \\ x \end{pmatrix}\right)$$

$$= \frac{x}{p} - \frac{(n-x)}{(1-p)} = 0 \ .$$

Then

$$x(1-p) - p(n-x) = 0 \text{ and } \hat{p}(x) = \frac{x}{n}$$

is the maximum likelihood estimator.

The maximum likelihood estimator may not be unique.
Let $X_1, X_2, \ldots, X_n$ be independent Uniform$(\theta - 1/2, \theta + 1/2)$ with

$$f_{X_i}(x_i|\theta) = I[\theta - 1/2 < x_i < \theta + 1/2] \text{ for } -\infty < \theta < \infty \ .$$

Then

$$L(\theta|x_1, x_2, \ldots x_n) = I[x_{(n)} - 1/2 < \theta < x_{(1)} + 1/2]$$

and $\hat{\theta}$ is any value between $X_{(n)} - 1/2$ and $X_{(1)} + 1/2$.

The maximum likelihood estimator may not exist.
Let $X_1, X_2, \ldots, X_n$ be independent with density

$$f_{X_i}(x_i|\theta) = (1-\lambda)\frac{e^{-(x_i-\mu)^2/2}}{\sqrt{2\pi}} + \lambda\frac{e^{-(x_i-\mu)^2/(2\sigma^2)}}{\sigma\sqrt{2\pi}}$$

for $\theta = (\mu, \sigma^2) \in \{\theta : -\infty < \mu < \infty, \sigma^2 > 0\}$ with λ known. For $\mu = x_1$ the likelihood

$$L(\theta|x_1, x_2, \ldots, x_n) = \prod_{i=1}^{n} f_{X_i}(x_i|\theta) = \left(\frac{(1-\lambda)}{\sqrt{2\pi}} + \frac{\lambda}{\sigma\sqrt{2\pi}}\right)\prod_{i=2}^{n} f_{X_i}(x_i|\theta) \to \infty$$

as $\sigma^2 \to 0$.

The maximum likelihood estimator may not be **consistent**.

Definition 11.2 *A consistent estimator $\hat{\theta}(X_1, X_2, \ldots, X_n)$ for θ satisfies*

$$P(|\hat{\theta}(X_1, X_2, \ldots, X_n) - \theta| > \varepsilon) \to 0 \text{ as } n \to \infty$$

for any $\varepsilon > 0$. That is, we have convergence in probability:

$$\hat{\theta}(X_1, X_2, \ldots, X_n) \xrightarrow{p} \theta \text{ as } n \to \infty.$$

For example, let X_i, Y_i both be independent $\mathcal{N}(\mu_i, \sigma^2)$ for $i = 1, 2, \ldots, n$. The maximum likelihood estimator for σ^2 is

$$\hat{\sigma}^2 = \frac{\sum_{i=1}^{n}(X_i - Y_i)^2}{4n} = \frac{2\sigma^2\chi_n^2}{4n} \xrightarrow{p} \frac{\sigma^2}{2}$$

using $E(\hat{\sigma}^2) = \sigma^2/2$, $\mathrm{Var}(\hat{\sigma}^2) = \sigma^4/(2n)$ and Chebyshev's theorem.

11.6.1 Properties of Maximum Likelihood Estimators

Invariance under transformations.
Suppose we have a 1-1 transformation $\xi = g(\theta)$ of the parameter θ. If we write

$$L^*(\xi|\mathbf{x}) = L(g^{-1}(\xi)|\mathbf{x})$$

then if $\hat{\theta}$ maximizes $L(\theta|\mathbf{x})$ then $\hat{\xi} = g(\hat{\theta})$ maximizes $L^*(\xi|\mathbf{x})$ since

$$\sup_{\xi} L^*(\xi|\mathbf{x}) = \sup_{\xi} L(g^{-1}(\xi)|\mathbf{x}) = \sup_{\theta} L(\theta|\mathbf{x}) = L(\hat{\theta}|\mathbf{x}) = L^*(g(\hat{\theta})|\mathbf{x}) \ .$$

If the function $\xi = g(\theta)$ is not 1-1, then we define the **induced likelihood** by

$$L^*(\xi|\mathbf{x}) = \sup_{\theta:g(\theta)=\xi} L(\theta|\mathbf{x}) \ .$$

We then have the following

Theorem 11.9 *If $\hat{\theta}$ is the maximum likelihood estimator of θ, then for any function $g(\theta)$, the maximum likelihood estimator of $g(\theta)$ is $g(\hat{\theta})$.*

Proof.

$$L^*(\hat{\xi}|\mathbf{x}) = \sup_{\xi} L^*(\xi|\mathbf{x}) = \sup_{\xi} \sup_{\theta:g(\theta)=\xi} L(\theta|\mathbf{x}) = L(\hat{\theta}|\mathbf{x}) \ .$$

Furthur,

$$L(\hat{\theta}|\mathbf{x}) = \sup_{\theta:g(\theta)=g(\hat{\theta})} L(\theta|\mathbf{x}) = L^*(g(\hat{\theta})|\mathbf{x}) \ .$$

From these we get $L^*(\hat{\xi}|\mathbf{x}) = L^*(g(\hat{\theta})|\mathbf{x})$ and we can take $\hat{\xi} = g(\hat{\theta})$ to maximize.■

Sufficiency.

Generally, the maximum likelihood estimator is a function of the sufficient statistic.

Lemma 11.4 *If the maximum likelihood estimator $\hat{\theta}(\mathbf{x})$ exists and is unique, and if $\mathbf{T}(\mathbf{x})$ is a sufficient statistic, then $\hat{\theta}(\mathbf{x})$ is a function of $\mathbf{T}(\mathbf{x})$.*

Proof.

Using the Neyman-Fisher factorization theorem,

$$L(\theta|\mathbf{x}) = g(\mathbf{T}(\mathbf{x}), \theta)h(\mathbf{x}) \ .$$

Thus $\sup_\theta L(\theta|\mathbf{x})$ is equivalent to $\sup_\theta g(\mathbf{T}(\mathbf{x}), \theta)$ and $\hat{\theta}$ is a function of $\mathbf{T}(\mathbf{x})$.■

When the maximum likelihood estimator is not unique, m.l.e.'s can be constructed that are not finctions of the sufficient statistic. For example, if $X_1, X_2, \ldots, X_n$ are independent Uniform$(\theta - 1/2, \theta + 1/2)$ then

$$\frac{1}{(1+X_1^2)}(X_{(n)} - 1/2) + \frac{X_1^2}{(1+X_1^2)}(X_{(1)} + 1/2)$$

maximizes but is a function of X_1 as well as the sufficient statistics

$$X_{(1)} = \min\{X_i\}, \text{ and } X_{(n)} = \max\{X_i\} \ .$$

However, we can always select a m.l.e. that is a function of the sufficient statistic. In the previous example we could take

$$\hat{\theta} = (X_{(1)} + X_{(n)})/2 \ .$$

Maximum likelihood estimators as solutions to likelihood derivative equations.
Define the log likelihood function

$$\mathcal{L}(\theta|\mathbf{x}) = \ln(L(\theta|\mathbf{x})) \ .$$

We have the following

Theorem 11.10 *If the parameter space Θ is an open set in R^k, $\ddot{\mathcal{L}}(\theta|\mathbf{x})$ exists and is continuous, then sufficient conditions for $\hat{\theta}$ to be a* **local maximum** *are*

$$\dot{\mathcal{L}}(\hat{\theta}|\mathbf{x}) = \left(\frac{\partial \mathcal{L}(\theta|\mathbf{x})}{\partial \theta}\right)^{K\times 1}|_{\theta=\hat{\theta}} = \mathbf{0}^{K\times 1}$$

and

$$-\ddot{\mathcal{L}}(\hat{\theta}|\mathbf{x}) = -\left(\frac{\partial^2 \mathcal{L}(\theta|\mathbf{x})}{\partial\theta\partial\theta^T}\right)^{K\times K}|_{\theta=\hat{\theta}} \ \textit{is positive definite.}$$

Note, positive definite means

$$-\mathbf{a}^T\ddot{\mathcal{L}}(\hat{\theta}|\mathbf{x})\mathbf{a} > 0 \text{ for } \mathbf{a}^{K\times 1} \neq \mathbf{0}^{K\times 1} \ .$$

Proof.
Write the univariate function $g(\lambda) = \mathcal{L}(\theta + \lambda\mathbf{a}|\mathbf{x})$ for $\lambda \in [0,1]$. Then using a Taylor expansion

$$g(\lambda) = g(0) + \lambda g'(0) + \frac{\lambda^2}{2}g''(\xi)$$

where $\xi \in [0,\lambda]$ and $\mathbf{a} = (a_1, a_2, \ldots, a_K)$. Since

$$g'(\lambda) = \sum_{k=1}^{K} a_k \frac{\partial \mathcal{L}(\theta + \lambda\mathbf{a}|\mathbf{x})}{\partial \theta_k} = \mathbf{a}^T\dot{\mathcal{L}}(\theta + \lambda\mathbf{a}|\mathbf{x})$$

and

$$g''(\xi) = \sum_{j=1}^{K}\sum_{k=1}^{K} a_j a_k \frac{\partial^2 \mathcal{L}(\theta + \xi\mathbf{a}|\mathbf{x})}{\partial\theta_j\partial\theta_k} = \mathbf{a}^T\ddot{\mathcal{L}}(\theta + \xi\mathbf{a}|\mathbf{x})\mathbf{a}$$

we have setting $\lambda = 1$

$$\mathcal{L}(\hat{\theta} + \mathbf{a}|\mathbf{x}) = \mathcal{L}(\hat{\theta}|\mathbf{x}) + \mathbf{a}^T \dot{\mathcal{L}}(\hat{\theta}|\mathbf{x}) + \frac{1}{2}\mathbf{a}^T \ddot{\mathcal{L}}(\hat{\theta} + \xi\mathbf{a}|\mathbf{x})\mathbf{a}$$

where $\xi \in [0, 1]$. Since $\dot{\mathcal{L}}(\hat{\theta}|\mathbf{x}) = \mathbf{0}$ and for $\mathbf{a} \neq \mathbf{0}$ sufficiently small

$$\mathbf{a}^T \ddot{\mathcal{L}}(\hat{\theta} + \xi\mathbf{a}|\mathbf{x})\mathbf{a} < 0$$

by the positive definite condition and continuity, we have

$$\mathcal{L}(\hat{\theta} + \mathbf{a}|\mathbf{x}) < \mathcal{L}(\hat{\theta}|\mathbf{x})$$

and a relative maximum occurs at $\hat{\theta}$. ■

For an example, let $\mathbf{X} = (X_1, X_2, \ldots, X_K)$ and

$$P(\mathbf{X} = \mathbf{x}) = \frac{n!}{x_1! x_2! \cdots x_K!} p_1^{x_1} p_2^{x_2} \cdots p_K^{x_K}$$

where $\sum_{k=1}^K x_k = n$ and $p_k > 0$, $\sum_{k=1}^K p_k = 1$. Define

$$\theta_k = \ln(p_k/p_K) \text{ for } k = 1, 2, \ldots, K-1 \ .$$

Then

$$p_k(\theta) = \frac{e^{\theta_k}}{1 + \sum_{j=1}^{K-1} e^{\theta_j}} \text{ and } p_K(\theta) = 1 - \sum_{j=1}^{K-1} p_j = \frac{1}{1 + \sum_{j=1}^{K-1} e^{\theta_j}} \ .$$

We have

$$\mathcal{L}(\theta|\mathbf{x}) = \sum_{k=1}^{K-1} x_k \theta_k - n \ln(1 + \sum_{j=1}^{K-1} e^{\theta_j}) + \ln(n!) - \sum_{k=1}^{K} \ln(x_k!)$$

and

$$\frac{\partial \mathcal{L}(\theta|\mathbf{x})}{\partial \theta_k} = x_k - \frac{n e^{\theta_k}}{1 + \sum_{j=1}^{K-1}} = x_k - n p_k = 0 \text{ for } k = 1, 2, \ldots K-1 \ .$$

From this

$$p_k(\hat{\theta}) = \frac{x_k}{n} \text{ for } k = 1, 2, \ldots K$$

is the unique solution since

$$-\ddot{\mathcal{L}}(\theta|\mathbf{x}) = n \begin{pmatrix} p_1(1-p_1) & -p_1p_2 & \dots & -p_1p_{K-1} \\ -p_2p_1 & p_2(1-p_2) & \dots & -p_2p_{K-1} \\ \vdots & \vdots & \ddots & \vdots \\ -p_{K-1}p_1 & -p_{K-1}p_2 & \dots & p_{K-1}(1-p_{K-1}) \end{pmatrix}$$

is positive definite everywhere (not just at $\hat{\theta}$) since

$$-\mathbf{a}^T\ddot{\mathcal{L}}(\theta|\mathbf{x})\mathbf{a} = n(\sum_{k=1}^{K-1} a_k^2 p_k - (\sum_{k=1}^{K-1} a_k p_k)^2) > 0$$

for $\mathbf{a} \neq \mathbf{0}$.

Another example is the general exponential family with natural parameter $\eta = (\eta_1, \eta_2, \dots, \eta_K)^T$ and density with respect to a measure $\mu(\mathbf{x})$ given by

$$f_{\mathbf{X}}(\mathbf{x}|\eta) = C(\eta)\exp\{\sum_{i=1}^{K} T_i(\mathbf{x})\eta_i\}h(\mathbf{x}) \ .$$

The log likelihood can be written

$$\mathcal{L}(\eta|\mathbf{x}) = \eta^T\mathbf{T}(x) - A(\eta) + \ln(h(\mathbf{x}))$$

where $A(\eta) = -\ln(C(\eta))$. The derivative equation is

$$\dot{\mathcal{L}}(\eta|\mathbf{x}) = \frac{\partial\mathcal{L}(\eta|\mathbf{x})}{\partial\eta} = \mathbf{T}(\mathbf{x}) - \frac{\partial A(\eta)}{\partial\eta} = \mathbf{0}^{K\times 1}$$

and

$$-\ddot{\mathcal{L}}(\eta|\mathbf{x}) = \frac{\partial^2 A(\eta)}{\partial\eta\partial\eta^T} = Cov(\mathbf{T}(\mathbf{X}))$$

is positive definite everywhere. We also have

$$E_\eta(\mathbf{T}(\mathbf{X})) = \frac{\partial A(\eta)}{\partial\eta}$$

so the m.l.e. $\hat{\eta}$ satisfies

$$\mathbf{T}(\mathbf{x}) = E_{\hat{\eta}}(\mathbf{T}(\mathbf{X})) \ .$$

A particular case is a sample from a bivariate normal where

$$\mathbf{X}_i = \begin{pmatrix} X_{i1} \\ X_{i2} \end{pmatrix} \ : \ \mathcal{N}_2\left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}\right)$$

are independent vectors for $i = 1, 2, \ldots, n$. The log likelihood is

$$\mathcal{L}(\eta|\mathbf{x}) = \ln \prod_{i=1}^{n} \frac{1}{\sigma_1\sigma_2\sqrt{1-\rho^2}2\pi} \times$$

$$\exp\left\{ \frac{-1}{2(1-\rho^2)} \left[\left(\frac{x_{i1}-\mu_1}{\sigma_1}\right)^2 - 2\rho\left(\frac{x_{i1}-\mu_1}{\sigma_1}\right)\left(\frac{x_{i2}-\mu_2}{\sigma_2}\right) + \left(\frac{x_{i2}-\mu_2}{\sigma_2}\right)^2 \right] \right\} .$$

Then

$$\mathbf{T}(\mathbf{x}) = (\sum_{i=1}^{n} x_{i1}, \sum_{i=1}^{n} x_{i2}, \sum_{i=1}^{n} x_{i1}^2, \sum_{i=1}^{n} x_{i1}x_{i2}, \sum_{i=1}^{n} x_{i2}^2)^T$$

$$\eta = \left(\frac{\mu_1 - \mu_2\rho\sigma_1/\sigma_2}{(1-\rho^2)\sigma_1^2}, \ \frac{\mu_2 - \mu_1\rho\sigma_2/\sigma_1}{(1-\rho^2)\sigma_2^2}, \ \frac{-1}{2(1-\rho^2)\sigma_1^2}, \ \frac{\rho}{(1-\rho^2)\sigma_1\sigma_2}, \ \frac{-1}{2(1-\rho^2)\sigma_2^2} \right)^T$$

and

$$E_\eta(\mathbf{T}(\mathbf{X})) = (n\mu_1, \ n\mu_2, \ n(\sigma_1^2+\mu_1^2), \ n(\rho\sigma_1\sigma_2+\mu_1\mu_2), \ n(\sigma_2^2+\mu_2^2))^T .$$

Solving the equation $\mathbf{T}(\mathbf{x}) = E_{\hat{\eta}}(\mathbf{T}(\mathbf{X}))$ gives

$$\hat{\mu}_1 = \frac{\sum_{i=1}^n x_{i1}}{n} = \bar{x}_1, \ \hat{\mu}_2 = \frac{\sum_{i=1}^n x_{i2}}{n} = \bar{x}_2, \tag{11.4}$$

$$\hat{\sigma_1}^2 = \frac{\sum_{i=1}^n (x_{i1}-\bar{x}_1)^2}{n}, \ \hat{\sigma_2}^2 = \frac{\sum_{i=1}^n (x_{i2}-\bar{x}_2)^2}{n}, \ \hat{\rho} = \frac{\sum_{i=1}^n (x_{i1}-\bar{x}_1)(x_{i2}-\bar{x}_2)}{n\hat{\sigma_1}\hat{\sigma_2}} .$$

For a multivariate generalization, let $\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}$ be independent multivariate normal $\mathcal{N}_p(\mu, \Sigma)$ where

$$\mu = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_p \end{pmatrix}, \ \Sigma = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \ldots & \sigma_{1p} \\ \sigma_{21} & \sigma_{22} & \ldots & \sigma_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{p1} & \sigma_{p2} & \ldots & \sigma_{pp} \end{pmatrix} = (\sigma_{ij})$$

with Σ symmetric, positive definite. The joint density is

$$f_{\mathbf{X_1},\mathbf{X_2},\ldots,\mathbf{X_n}}(\mathbf{x_1},\mathbf{x_2},\ldots,\mathbf{x_n}|\eta) = \prod_{i=1}^{n} \frac{1}{(2\pi)^{p/2}|\Sigma|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}_i-\mu)^T\Sigma^{-1}(\mathbf{x}_i-\mu)\right\}$$

and the log likelihood is

$$\mathcal{L}(\eta|\mathbf{x_1},\mathbf{x_2},\ldots,\mathbf{x_n}) = -\frac{np}{2}\ln(2\pi) - \frac{n}{2}\ln(|\Sigma|) - \frac{1}{2}\sum_{i=1}^{n}(\mathbf{x}_i-\mu)^T\Sigma^{-1}(\mathbf{x}_i-\mu)$$

$$= -\frac{np}{2}\ln(2\pi) - \frac{n}{2}\ln(|\Sigma|) - \frac{n}{2}\sum_{j=1}^{p}\sum_{k=1}^{p}\mu_j\sigma^{jk}\mu_k$$

$$-\sum_{j=1}^{p}\frac{\sigma^{jj}}{2}(\sum_{i=1}^{n}x_{ij}^2) - \sum_{j=1}^{p-1}\sum_{k=j+1}^{p}\sigma^{jk}(\sum_{i=1}^{n}x_{ij}x_{ik}) + \sum_{j=1}^{p}(\sum_{k=1}^{p}\mu_k\sigma^{jk})\sum_{i=1}^{n}x_{ij}$$

where $\Sigma^{-1} = (\sigma^{ij}) = (\sigma^{ji})$ is also symmetric. This is in the exponential family with dimension $K = 2p + p(p-1)/2$ and

$$\mathbf{T}(\mathbf{x}) = (\sum_{i=1}^{n}x_{i1}^2,\ldots,\sum_{i=1}^{n}x_{ip}^2,\sum_{i=1}^{n}x_{i1}x_{i2},\ldots,\sum_{i=1}^{n}x_{i(p-1)}x_{ip},\sum_{i=1}^{n}x_{i1},\ldots,\sum_{i=1}^{n}x_{ip})^T$$

$$\eta = \left(\frac{-\sigma^{11}}{2},\ldots,\frac{-\sigma^{pp}}{2},\sigma^{12},\ldots,\sigma^{(p-1)p},\sum_{j=1}^{p}\mu_j\sigma^{j1},\ldots,\sum_{j=1}^{p}\mu_j\sigma^{jp}\right)^T$$

$$E_\eta(\mathbf{T}(\mathbf{X})) =$$

$$(n(\sigma_{11}+\mu_1^2),\ldots,n(\sigma_{pp}+\mu_p^2),n(\sigma_{12}+\mu_1\mu_2),\ldots,n(\sigma_{(p-1)p}+\mu_{(p-1)}\mu_p),n\mu_1,\ldots,n\mu_p)^T .$$

Solving the equation $\mathbf{T}(\mathbf{x}) = E_{\hat{\eta}}(\mathbf{T}(\mathbf{X}))$ gives m.l.e.

$$\hat{\mu}_j = \frac{\sum_{i=1}^{n}x_{ij}}{n} = \bar{x}_j \quad \text{for } j = 1,2,\ldots,p$$

$$\hat{\sigma}_{jj} = \frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)^2 \quad \text{for } j = 1,2,\ldots,p$$

$$\hat{\sigma}_{jk} = \frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\bar{x}_j)(x_{ik}-\bar{x}_k) \quad \text{for } 1 \le j < k \le p.$$

Consistency of the m.l.e.

Theorem 11.11 *Let $\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}$ be a sequence of independent identically distributed random vectors with c.d.f. $F(\mathbf{x}|\theta)$, $\theta \in \Theta$ a parameter space that is a compact subset of R^K. Let the family of distributions be dominated by a sigma finite measure $\mu(\mathbf{x})$ and let $f(\mathbf{x}|\theta) = dF(\mathbf{x}|\theta)/d\mu$ be the density with respect to $\mu(\mathbf{x})$. Assume*

(a) $\ln(f(\mathbf{x}|\theta))$ *is measurable in* $\mathbf{x}$ *for each* $\theta \in \Theta$ *and equicontinuous in* θ,

(b) *there exists an* $\mathbf{x}$ *measurable function* $G(\mathbf{x})$ *such that*

$$|\ln(f(\mathbf{x}|\theta))| \leq G(\mathbf{x}) \text{ where } \int_{\mathcal{X}} G(\mathbf{x}) dF(\mathbf{x}|\theta) < \infty \ .$$

If $\hat{\theta}_n$ is any value that maximizes

$$\mathcal{L}_n(\theta|\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n}) = \sum_{i=1}^{n} \ln(f(\mathbf{x}_i|\theta))$$

then the m.l.e. $\hat{\theta}_n$ is a strongly consistent estimator:

$$\hat{\theta}_n \xrightarrow{a.s.} \theta_0$$

where θ_0 is the true value of the parameter.

Proof.
Using Rubin's uniform strong law of large numbers (theorem 9.12) we have

$$\frac{1}{n}\mathcal{L}_n(\theta|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}) = \frac{1}{n}\sum_{i=1}^{n} \ln(f(\mathbf{X}_i|\theta)) \xrightarrow{a.s.} E_{\theta_0}(\ln(f(\mathbf{X}|\theta)) \ .$$

Applying Jensen's inequality (theorem 5.2) gives

$$E_{\theta_0}(\ln\left(\frac{f(\mathbf{X}|\theta)}{f(\mathbf{X}|\theta_0)}\right)) = \int \ln\left(\frac{f(\mathbf{x}|\theta)}{f(\mathbf{x}|\theta_0)}\right) f(\mathbf{x}|\theta_0) d\mu(\mathbf{x}) \leq \ln\left(\int \frac{f(\mathbf{x}|\theta)}{f(\mathbf{x}|\theta_0)} f(\mathbf{x}|\theta_0) d\mu(\mathbf{x})\right)$$

$$\leq \ln\left(\int f(\mathbf{x}|\theta) d\mu(\mathbf{x})\right) = \ln(1) = 0$$

with equality if and only if $f(\mathbf{x}|\theta) = f(\mathbf{x}|\theta_0)$ a.e. μ. Thus

$$E_{\theta_0}(\ln(f(\mathbf{X}|\theta)) \leq E_{\theta_0}(\ln(f(\mathbf{X}|\theta_0))$$

with equality if and only if $f(\mathbf{x}|\theta) = f(\mathbf{x}|\theta_0)$ a.e. μ. Since the limit function is continuous (by theorem 9.12), has a unique maximum at θ_0, and Θ is compact, the expected value is bounded away from its maximum when θ is bounded away from θ_0. Thus for $\delta > 0$ there exists an $\varepsilon > 0$ such that

$$E_{\theta_0}(\ln(f(\mathbf{X}|\theta)) \leq E_{\theta_0}(\ln(f(\mathbf{X}|\theta_0)) - \varepsilon \tag{11.5}$$

for $||\theta - \theta_0|| \geq \delta$.
Now assume to the contrary that there exists a set of positive probability in the space of points $\mathbf{x}^\infty = (\mathbf{x_1}, \mathbf{x_2}, \ldots)$ where $\hat{\theta}_n(\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n})$ does not converge to θ_0. Then there exists a subsequence $\{m\} \subset \{n\}$ and a limit point $\theta_{\mathbf{x}^\infty}$ such that

$$\hat{\theta}_m \to \theta_{\mathbf{x}^\infty} \text{ where } \theta_{\mathbf{x}^\infty} \neq \theta_0 \ .$$

Because $\hat{\theta}_m$ produces a maximum for every m

$$\frac{1}{m}\sum_{i=1}^{m} \ln(f(\mathbf{x}_i|\hat{\theta}_m)) \geq \frac{1}{m}\sum_{i=1}^{m} \ln(f(\mathbf{x}_i|\theta_0)) \ .$$

By uniform convergence and continuity of the limit

$$E_{\theta_0}(\ln(f(\mathbf{X}|\theta)|_{\theta=\theta_{\mathbf{x}^\infty}}) \geq E_{\theta_0}(\ln(f(\mathbf{X}|\theta_0))$$

which contradicts equation (11.5). Thus $\hat{\theta}_n$ is strongly consistent. ■

Limiting normal distribution of the m.l.e. Let $f(\mathbf{x}|\theta)$ for $\theta \in \Theta$ be densities with respect to a measure $\mu(\mathbf{x})$.
Consider the following assumptions:
Assumption 1. $\ln(f(\mathbf{x}|\theta))$ *is measurable in* $\mathbf{x}$ *for each* $\theta \in \Theta$ *and equicontinuous in* θ.
Assumption 2. *There exists an* $\mathbf{x}$ *measurable function* $G(\mathbf{x})$ *such that*

$$|\ln(f(\mathbf{x}|\theta))| \leq G(\mathbf{x}) \text{ where } \int_{\mathcal{X}} G(\mathbf{x}) f(\mathbf{x}|\theta) d\mu(\mathbf{x}) < \infty \ .$$

Assumption 3. *There exists an open subset* $V_\varepsilon(\theta_0)$ *of* Θ *containing the true parameter* θ_0 *such that for almost all* $\mathbf{x}$*, independent of* θ*, the density has all (measurable in* $\mathbf{x}$) first and second order partial derivatives with respect to the components of $\theta \in V_\varepsilon(\theta_0)$.
Assumption 4. *The first order partial derivatives of* $\ln(f(\mathbf{x}|\theta))$ *satisfy*

$$E_\theta\left(\frac{\partial \ln(f(\mathbf{X}|\theta))}{\partial\theta}\right) = \frac{\partial}{\partial\theta} E_\theta(\ln(f(\mathbf{X}|\theta))) = \mathbf{0}^{K\times 1}$$

and the positive definite information matrix satisfies

$$\mathcal{I}(\theta) = -E_\theta\left(\frac{\partial^2 \ln(f(\mathbf{X}|\theta))}{\partial\theta\partial\theta^T}\right) = E_\theta\left(\frac{\partial \ln(f(\mathbf{X}|\theta))}{\partial\theta}\frac{\partial \ln(f(\mathbf{X}|\theta))}{\partial\theta^T}\right) .$$

Assumption 5. *For $\theta_0 \in \Theta$ there exists an $\mathbf{x}$ measurable function $H(\mathbf{x})$ such that*

$$\left|\left|\left.\frac{\partial^2 \ln(f(\mathbf{x}|\theta))}{\partial\theta\partial\theta^T}\right|_{\theta_0}\right|\right| \leq H(\mathbf{x}), \quad \int_{\mathcal{X}} H(\mathbf{x}) f(\mathbf{x}|\theta_0) d\mu(\mathbf{x}) < \infty$$

and

$$\frac{\partial^2 \ln(f(\mathbf{x}|\theta))}{\partial\theta\partial\theta^T}$$

is measurable in $\mathbf{x}$ and equicontinuous in θ.

Theorem 11.12 *Let $\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}$ be independent identically distributed random vectors with density $f(\mathbf{x}|\theta)$, $\theta \in \Theta$, with respect to a measure $\mu(\mathbf{x})$ satisfying assumptions (1) through (5) with Θ an open subset of a compact subset of R^K. If the maximum likelihood estimator $\hat{\theta}_n$ satisfies the derivative equation*

$$\dot{\mathcal{L}}(\hat{\theta}_n|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}) = \mathbf{0}^{K\times 1}$$

then, as $n \to \infty$,

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \xrightarrow{d} \mathbf{Z} : \mathcal{N}_K(\mathbf{0}, \mathcal{I}^{-1}(\theta_0)) .$$

Proof.
Assumptions (1) and (2) give a.s. consistency of the m.l.e. by theorem (11.11). Using assumption (3) and expanding $\dot{\mathcal{L}}(\hat{\theta}_n|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n})$ in a Taylor series about θ_0 we get

$$\frac{1}{\sqrt{n}}\dot{\mathcal{L}}(\hat{\theta}_n|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}) = \frac{1}{\sqrt{n}}\dot{\mathcal{L}}(\theta_0|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n})$$

$$+ \int_0^1 \frac{1}{n}\ddot{\mathcal{L}}(\theta_0 + \eta(\hat{\theta}_n - \theta_0)|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}) d\eta \sqrt{n}(\hat{\theta}_n - \theta_0) .$$

Since the left side is zero, ($\hat{\theta}_n$ is a root of the derivative equation), we have

$$\frac{1}{\sqrt{n}}\dot{\mathcal{L}}(\theta_0|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}) = \int_0^1 (-\frac{1}{n}\ddot{\mathcal{L}}(\theta_0 + \eta(\hat{\theta}_n - \theta_0)|\mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n})) d\eta \sqrt{n}(\hat{\theta}_n - \theta_0) .$$

Taking the limit as $n \to \infty$

$$\mathbf{Z} = \int_0^1 \mathcal{I}(\theta_0) d\eta \lim_n \sqrt{n}(\hat{\theta}_n - \theta_0) \ .$$

Here the limit in distribution

$$\mathbf{Z} = \lim_n \frac{1}{\sqrt{n}} \dot{\mathcal{L}}(\theta_0 | \mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}) : \mathcal{N}_K(\mathbf{0}, \mathcal{I}(\theta_0))$$

using the central limit theorem and assumption (4). Using assumption (5), $\hat{\theta}_n \xrightarrow{a.s.} \theta_0$, uniform equicontinuity of $\ddot{\mathcal{L}}(\theta | \mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n})$ on the open subset Θ of a compact subset of R^K (since a continuous function on a compact set is uniformly continuous), theorem (9.4), and Rubin's strong law of large numbers (theorem 9.12) we have

$$-\frac{1}{n} \ddot{\mathcal{L}}(\theta_0 + \eta(\hat{\theta}_n - \theta_0) | \mathbf{X_1}, \mathbf{X_2}, \ldots, \mathbf{X_n}) \xrightarrow{a.s.} \mathcal{I}(\theta_0) \ .$$

Thus

$$\mathcal{I}(\theta_0) \lim_n \sqrt{n}(\hat{\theta}_n - \theta_0) = \mathbf{Z}$$

and inverting the positive definite $\mathcal{I}(\theta_0)$ (assumption (4)) gives

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \xrightarrow{d} \mathcal{I}^{-1}(\theta_0) \mathbf{Z} : \mathcal{N}_K(\mathbf{0}, \mathcal{I}^{-1}(\theta_0)) \ . \blacksquare$$

We note the components asymptotically attain the information lower bound for unbiased estimators. However, for finite n the exact variance-covariance matrix could be infinite.

As an example, let

$$\mathbf{X}_i = \begin{pmatrix} X_{i1} \\ X_{i2} \end{pmatrix} : \mathcal{N}_2 \left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} \right) \text{ for } i = 1, 2, \ldots, n$$

be independent bivariate normal with $\theta = (\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \rho)^T \in \Theta$ where

$$\Theta = \{(\mu_1, \mu_2, \sigma_1^2, \sigma_2^2, \rho)^T : -\infty < a_{j1} < \mu_j < a_{j2} < \infty, \ \ 0 < b_{j1} < \sigma_j^2 < b_{j2} < \infty,$$

$$-1 < c_1 < \rho < c_2 < 1, \ \ j = 1, 2\} \ .$$

The m.l.e. (from equations (11.4))

$$\hat{\theta}_n = \begin{pmatrix} \hat{\mu}_1 \\ \hat{\mu}_2 \\ \hat{\sigma}_1^2 \\ \hat{\sigma}_2^2 \\ \hat{\rho} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n X_{i1}/n \\ \sum_{i=1}^n X_{i2}/n \\ \sum_{i=1}^n (X_{i1} - \bar{X}_1)^2/n \\ \sum_{i=1}^n (X_{i2} - \bar{X}_2)^2/n \\ \sum_{i=1}^n (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2)/(n\hat{\sigma}_1\hat{\sigma}_2) \end{pmatrix}$$

where $\bar{X}_j = \sum_{i=1}^n X_{ij}/n$ for $j = 1, 2$, satisfies as $n \to \infty$

$$\sqrt{n}(\hat{\theta}_n - \theta_0) \xrightarrow{d} \mathbf{Z} : \mathcal{N}_5(\mathbf{0}, \mathcal{I}^{-1}(\theta_0))$$

for the true value $\theta_0 \in \Theta$ and $\mathcal{I}(\theta) =$

$$\frac{1}{(1-\rho^2)} \begin{pmatrix} 1/\sigma_1^2 & -\rho/(\sigma_1\sigma_2) & 0 & 0 & 0 \\ -\rho/(\sigma_1\sigma_2) & 1/\sigma_2^2 & 0 & 0 & 0 \\ 0 & 0 & (2-\rho^2)/(4\sigma_1^4) & -\rho^2/(4\sigma_1^2\sigma_2^2) & -\rho/(2\sigma_1^2) \\ 0 & 0 & -\rho^2/(4\sigma_1^2\sigma_2^2) & (2-\rho^2)/(4\sigma_2^4) & -\rho/(2\sigma_2^2) \\ 0 & 0 & -\rho/(2\sigma_1^2) & -\rho/(2\sigma_2^2) & (1+\rho^2)/(1-\rho^2) \end{pmatrix},$$

$$\mathcal{I}^{-1}(\theta) = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 & 0 & 0 & 0 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 & 0 & 0 & 0 \\ 0 & 0 & 2\sigma_1^4 & 2\rho^2\sigma_1^2\sigma_2^2 & \rho(1-\rho^2)\sigma_1^2 \\ 0 & 0 & 2\rho^2\sigma_1^2\sigma_2^2 & 2\sigma_2^4 & \rho(1-\rho^2)\sigma_2^2 \\ 0 & 0 & \rho(1-\rho^2)\sigma_1^2 & \rho(1-\rho^2)\sigma_2^2 & (1-\rho^2)^2 \end{pmatrix}.$$

Theorem 11.13 The Delta Method.
If $\sqrt{n}(\mathbf{X}_n - \mu) \xrightarrow{d} \mathcal{N}_p(\mathbf{0}, \Sigma)$ *and* $\mathbf{g}(\mathbf{x})^{K\times 1}$ *has continuous derivatives,* $K \le p$*, then*

$$\sqrt{n}(\mathbf{g}(\mathbf{X_n}) - \mathbf{g}(\mu)) \xrightarrow{d} \mathcal{N}_K(\mathbf{0}, \Lambda)$$

where

$$\Lambda = \left(\frac{\partial \mathbf{g}(\mu)}{\partial \mu^T}\right) \Sigma \left(\frac{\partial \mathbf{g}(\mu)^T}{\partial \mu}\right).$$

Proof.
Using a vector Taylor expansion

$$g(\mathbf{X}_n) = g(\mu) + \left(\frac{\partial g(\xi_n)}{\partial \mu^T}\right)(\mathbf{X}_n - \mu)$$

where ξ_n is between $\mathbf{X_n}$ and μ. Then

$$\sqrt{n}(\mathbf{g}(\mathbf{X}_n) - \mathbf{g}(\mu)) \xrightarrow{d} \left(\frac{\partial \mathbf{g}(\mu)}{\partial \mu^T}\right) \mathbf{Z}$$

where $\mathbf{Z} = \lim_n \sqrt{n}(\mathbf{X}_n - \mu) : \mathcal{N}_p(\mathbf{0}, \Sigma)$ since

$$\left(\frac{\partial \mathbf{g}(\xi_n)}{\partial \mu^T}\right) \xrightarrow{d} \left(\frac{\partial \mathbf{g}(\mu)}{\partial \mu^T}\right)$$

using theorem (9.6) since $\sqrt{n}(\mathbf{X}_n - \mu) \xrightarrow{d} \mathcal{N}_p(\mathbf{0}, \Sigma)$ gives $\mathbf{X}_n \xrightarrow{d} \mu$ and $\xi_n \xrightarrow{d} \mu$. The result follows from the linear transformation, -see section (10.3). ■

As an example of the use of this theorem, if

$$\sqrt{n}(\hat{\theta}_n - \theta) \xrightarrow{d} \mathbf{Z} : \mathcal{N}_K(\mathbf{0}, \mathcal{I}(\theta)^{-1})$$

then if $g = (g_1, g_2, \ldots, g_r)^T$ has continuous derivatives where $r \leq K$, we have

$$\sqrt{n}(g(\hat{\theta}_n) - g(\theta)) \xrightarrow{d} \mathbf{W} : \mathcal{N}_r(\mathbf{0}, \Lambda(\theta))$$

where

$$\Lambda(\theta)^{r\times r} = \left(\frac{\partial \mathbf{g}(\theta)}{\partial \theta^T}\right)^{r\times K} (\mathcal{I}(\theta)^{-1})^{K\times K} \left(\frac{\partial \mathbf{g}(\theta)^T}{\partial \theta}\right)^{K\times r} .$$

Applying this to $X_1, X_2, \ldots, X_n : \mathcal{N}(\mu, \sigma^2)$ we have for $\theta = (\mu, \sigma^2)^T$, the maximum likelihood estimators satisfy $\sqrt{n}(\hat{\theta}_n - \theta)$

$$= \sqrt{n} \begin{pmatrix} \bar{X} - \mu \\ \sum_{i=1}^n (X_i - \bar{X})^2/n - \sigma^2 \end{pmatrix} \xrightarrow{d} \mathbf{Z} : \mathcal{N}_2 \left(\begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1/\sigma^2 & 0 \\ 0 & 1/(2\sigma^4) \end{pmatrix}^{-1} \right)$$

where $\bar{X} = \sum_{i=1}^n X_i/n$. Then if $g(\theta) = \mu/\sigma$ we have

$$\sqrt{n} \left(\bar{X}/(\sum_{i=1}^n (X_i - \bar{X})^2/n)^{1/2} - \mu/\sigma \right) \xrightarrow{d} \mathbf{W} : \mathcal{N}_1(0, \lambda)$$

where

$$\lambda = (1/\sigma, -\mu/(2\sigma^3)) \begin{pmatrix} \sigma^2 & 0 \\ 0 & 2\sigma^4 \end{pmatrix} \begin{pmatrix} 1/\sigma \\ -\mu/(2\sigma^3) \end{pmatrix} = \left(1 + \frac{\mu^2}{2\sigma^2}\right) .$$

11.7 Bayes Point Estimators

We consider a distribution $\Lambda(\theta)$ over the parameter space Θ called the *prior* distribution. We introduce a loss function

$$L(\delta(\mathbf{X}), \theta) \geq 0$$

that measures the cost of estimating $g(\theta)$ using the estimator $\delta(\mathbf{X})$. The average or expected loss is called the risk function and we denote it by

$$R_\delta(\theta) = E_\theta(L(\delta(\mathbf{X}), \theta)) \ .$$

The Bayes risk of the estimator $\delta(\mathbf{X})$ is then the average of the risk with respect to the prior

$$r_\delta(\Lambda) = \int_{\theta \in \Theta} R_\delta(\theta) d\Lambda(\theta) \ .$$

The Bayes estimator $\delta_B(\mathbf{X})$ is an estimator that minimizes the Bayes risk. That is

$$r_{\delta_B}(\Lambda) = \int_{\theta \in \Theta} E_\theta(L(\delta_B(\mathbf{X}), \theta)) d\Lambda(\theta) \leq \int_{\theta \in \Theta} E_\theta(L(\delta(\mathbf{X}), \theta)) d\Lambda(\theta) = r_\delta(\Lambda)$$

for all $\delta(\mathbf{X})$.

For an example, let X have a binomial(n, p) distribution, let the loss for estimating $g(p) = p$ be squarred error

$$L(\delta(X), p) = (\delta(X) - p)^2$$

and consider the prior with density

$$\frac{d\Lambda(p)}{dp} = \lambda(p) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha - 1}(1 - p)^{\beta - 1} \text{ for } 0 < p < 1$$

where α, β are known. Then the Bayes estimator $\delta_B(X)$ minimizes

$$\int_0^1 \sum_{x=0}^{n} (\delta(x) - p)^2 \begin{pmatrix} n \\ x \end{pmatrix} p^x (1 - p)^{n - x} \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha - 1}(1 - p)^{\beta - 1} dp$$

$$= \sum_{x=0}^{n} \int_0^1 (\delta(x) - p)^2 \frac{\Gamma(n + \alpha + \beta)}{\Gamma(x + \alpha)\Gamma(n - x + \beta)} p^{x + \alpha - 1}(1 - p)^{n - x + \beta - 1} dp$$

$$\times \begin{pmatrix} n \\ x \end{pmatrix} \frac{\Gamma(x+\alpha)\Gamma(n-x+\beta)\Gamma(\alpha+\beta)}{\Gamma(n+\alpha+\beta)\Gamma(\alpha)\Gamma(\beta)} .$$

Thus the Bayes estimator is

$$\delta_B(x) = \int_0^1 p \frac{\Gamma(n+\alpha+\beta)}{\Gamma(x+\alpha)\Gamma(n-x+\beta)} p^{x+\alpha-1}(1-p)^{n-x+\beta-1} dp = E(p|x) = \frac{x+\alpha}{n+\alpha+\beta}$$

which is the mean of the *posterior* density

$$\lambda(p|x) = \frac{\Gamma(n+\alpha+\beta)}{\Gamma(x+\alpha)\Gamma(n-x+\beta)} p^{x+\alpha-1}(1-p)^{n-x+\beta-1} .$$

In general, for squarred error loss, the Bayes estimator is the posterior mean. If we can interchange the order of integration,

$$\int_{\theta\in\Theta}\int_{\mathcal{X}} (\delta(\mathbf{x})-g(\theta))^2 dF_{X|\theta}(\mathbf{x}|\theta) d\Lambda(\theta) = \int_{\mathcal{X}}\int_{\theta\in\Theta} (\delta(\mathbf{x})-g(\theta))^2 dF_{\theta|\mathbf{X}}(\theta|\mathbf{x}) dF_X(\mathbf{x})$$

and

$$\delta_B(\mathbf{x}) = \int_{\theta\in\Theta} g(\theta) dF_{\theta|X}(\theta|\mathbf{x})$$

minimizes. If the loss is absolute error $L(\delta(\mathbf{X}),\theta) = |\delta(\mathbf{X}) - g(\theta)|$ then the Bayes estimator is the median of the posterior distribution of $g(\theta)$.

A useful class of prior distributions is the conjugate[8] family that has the same form as the joint density of $\mathbf{X}|\theta$ but viewed as a function of θ. A way to derive the class is to write the joint density for fictitous sample values $\mathbf{x}^*$ then replace corresponding sufficient statistics $\mathbf{S}(\mathbf{x}^*)$ by parameters for the prior and then rescale so the prior integrates to 1.

For example, let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ where X_i are independent Poisson(θ) where $0 < \theta < \infty$. The joint density of a fictitious sample is

$$f_{\mathbf{X}^*}(\mathbf{x}^*|\theta) = \prod_{i=1}^{n^*} \frac{\theta^{x_i^*}}{x_i^*!} e^{-\theta} = \frac{\theta^{s^*} e^{-n^*\theta}}{\prod_{i=1}^{n^*} x_i^*!}$$

where $s^* = \sum_{i=1}^{n^*} x_i^*$. Setting $\alpha = s^*+1$, $1/\beta = n^*$, the conjugate prior family is

$$\lambda(\theta) = \frac{\theta^{\alpha-1} e^{-\theta/\beta}}{\Gamma(\alpha)\beta^\alpha} \text{ for } 0 < \theta < \infty$$

[8]Raiffa, Howard and Schlaiffer, Robert (1961) *Applied Statistical Decision Theory.* Cambridge: MIT Press.

which is the gamma(α, β) family.

For another example, let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ where X_i are independent $\mathcal{N}(\mu, \sigma^2)$. The joint density for a fictitious sample is

$$f_{\mathbf{X}^*}(\mathbf{x}^*|\mu, \sigma^2) = \frac{1}{(2\pi\sigma^2)^{n^*/2}} \exp\{-\sum_{i=1}^{n^*}(x_i^* - \mu)^2/(2\sigma^2)\}$$

which is proportional to

$$h^{n^*/2} e^{-n^* h(\mu - \bar{x}^*)^2/2} e^{-h(\sum x_i^{*2} - n^* \bar{x}^{*2})/2}$$

where $h = 1/\sigma^2$. Then a conjugate prior family for $\theta = (\mu, h)$ is

$$\lambda(\theta) = \frac{(\alpha h)^{1/2} e^{-\alpha h(\mu-\gamma)^2/2}}{\sqrt{2\pi}} \frac{h^{(\alpha+1)/2-1} e^{-h/(2\beta)}}{\Gamma((\alpha+1)/2)(2\beta)^{(\alpha+1)/2}}$$

setting $\alpha = n^*$, $1/\beta = \sum_{i=1}^{n^*} x_i^{*2} - n\bar{x}^{*2}$, $\gamma = \bar{x}^* = \sum_{i=1}^{n^*} x_i^*/n^*$. This is the normal-gamma(α, β, γ) family. That is, the prior density of μ given h is $\mathcal{N}(\gamma, 1/(\alpha h))$ and the marginal prior density of h is gamma$((\alpha+1)/2, 2\beta)$.

The nice feature of a conjugate prior is that the posterior ditribution belongs to the same class and the parameters of the posterior distribution (the conditional distribution of $\theta|\mathbf{X}$) can be obtained by identifying the sufficient statistics for the combined fictitous and observed sample $S(\mathbf{x}^*, \mathbf{x})$.

For the Poisson(θ) example, the posterior density for $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ is

$$\lambda(\theta|\mathbf{x}) = \frac{\theta^{\alpha'-1} e^{-\theta/\beta'}}{\beta'^{\alpha} \Gamma(\alpha')}$$

where $\alpha' = \alpha + \sum_{i=1}^{n} x_i$ and $1/\beta' = (1/\beta) + n$. The Bayes estimator for squarred error loss is then

$$\hat{\theta}_B(\mathbf{x}) = E(\theta|\mathbf{x}) = \alpha'\beta' = \frac{\alpha + \sum_{i=1}^{n} x_i}{\beta^{-1} + n} .$$

For the normal-gamma(α, β, γ) family, the posterior is also a normal-gamma$(\alpha', \beta', \gamma')$ family where

$$\alpha' = \alpha + n, \quad \frac{1}{\beta'} = \frac{1}{\beta} + (\sum_{i=1}^{n} x_i^2 - n\bar{x}^2) + \frac{n\alpha(\gamma - \bar{x})^2}{(n+\alpha)}, \quad \gamma' = \frac{(\alpha\gamma + n\bar{x})}{(\alpha + n)} .$$

The marginal distributions of μ and of $h = 1/\sigma^2$ are

$$\lambda(\mu) = \frac{\Gamma(\alpha/2+1)(\alpha\beta)^{1/2}}{\Gamma((\alpha+1)/2)\Gamma(1/2)(1+\alpha\beta(\mu-\gamma)^2)^{\alpha/2+1}} \text{ for } -\infty < \mu < \infty$$

$$\lambda(h) = \frac{h^{(\alpha+1)/2-1}e^{-h/(2\beta)}}{\Gamma((\alpha+1)/2)(2\beta)^{(\alpha+1)/2}} \text{ for } 0 < h < \infty \ .$$

For estimating μ using squarred error loss, the posterior mean gives

$$\hat{\mu}_B(\mathbf{x}) = E(\mu|\mathbf{x}) = \gamma' = \frac{(\alpha\gamma + n\bar{x})}{(\alpha+n)}$$

and for estimating σ^2 with squarred error loss

$$\hat{\sigma}^2_B(\mathbf{x}) = E(h^{-1}|\mathbf{x}) = \frac{1}{(\alpha'-1)\beta'} = \frac{1}{(\alpha+n-1)}\left(\frac{1}{\beta} + \sum_{i=1}^n x_i^2 - n\bar{x}^2 + \frac{n\alpha(\gamma-\bar{x})^2}{(n+\alpha)}\right) \ .$$

The binomial(n,p) has conjugate prior density

$$\lambda(p) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}p^{\alpha-1}(1-p)^{\beta-1} \text{ for } 0 < p < 1$$

which is a beta(α,β) density. The posterior is also a beta(α',β') where

$$\alpha' = \alpha + x, \quad \beta' = \beta + n - x \ .$$

For squarred error loss the Bayes estimator of p is

$$\hat{p}_B(x) = E(p|x) = \frac{\alpha'}{\alpha'+\beta'} = \frac{\alpha+x}{\alpha+\beta+n} \ . \tag{11.6}$$

If X:Hypergeometric(N,D,n) or for integer x,n,D,N, $x \le n, D \le N$,

$$P(X=x|D) = \frac{\binom{n}{x}\binom{N-n}{D-x}}{\binom{N}{D}} \text{ for } \max(0,n+D-N) \le x \le \min(n,D),$$

then a mathematically convenient family of priors for the parameter D with integer a,b known is for $d = 0,1,\ldots,N$

$$P(D=d) = \int_0^1 \binom{N}{d} p^d(1-p)^{N-d}\frac{\Gamma(a+b)}{\Gamma(a)\Gamma(b)}p^{a-1}(1-p)^{b-1}dp$$

$$= \frac{\begin{pmatrix} d+a-1 \\ a-1 \end{pmatrix}\begin{pmatrix} N-d+b-1 \\ b-1 \end{pmatrix}}{\begin{pmatrix} N+a+b-1 \\ a+b-1 \end{pmatrix}} = \begin{pmatrix} d+a-1 \\ d \end{pmatrix} \frac{(N)_d(a+b-1)_a}{(N+a+b-1)_{(a+d)}} \ . \tag{11.7}$$

If we call a negative hypergeometric(M, A, r) distribution for Y with

$$P(Y=y) = \begin{pmatrix} r+y-1 \\ y \end{pmatrix} \frac{(A)_r(M-A)_y}{(M)_{(r+y)}} \text{ for } y = 0, 1, \ldots, M-A,$$

which has expectation $r(M-A)/(A+1)$, then the prior for D is a negative hypergeometric$(N+a+b-1, a+b-1, a)$ prior with $E(D) = Na/(a+b)$. The posterior distribution is

$$P(D=d|x) = \frac{P(X=x|d)P(D=d)}{P(X=x)} =$$

$$\int_0^1 \begin{pmatrix} N-n \\ d-x \end{pmatrix} p^{d-x}(1-p)^{N-n-(d-x)} \frac{\Gamma(a+b+n)}{\Gamma(a+x)\Gamma(b+n-x)} p^{a+x-1}(1-p)^{b+(n-x)-1} dp$$

$$= \frac{\begin{pmatrix} d+a-1 \\ a+x-1 \end{pmatrix}\begin{pmatrix} N-d+b-1 \\ b+(n-x)-1 \end{pmatrix}}{\begin{pmatrix} N+a+b-1 \\ n+a+b-1 \end{pmatrix}}$$

$$= \begin{pmatrix} d+a-1 \\ d-x \end{pmatrix} \frac{(N-n)_{(d-x)}(n+a+b-1)_{(a+x)}}{(N+n+a+b-1)_{(a+d)}} \text{ for } d = x, x+1, \ldots, N-n+x$$

which is a negative hypergeometric$(N+n+a+b-1, n+a+b-1, a+x)$ for $D-x$. For squarred error loss, the Bayes estimator for D is

$$\hat{D}_B(x) = E(D|x) = x + \frac{(N-n)(a+x)}{(a+b+n)} = \frac{x(a+b+N)+a(N-n)}{(a+b+n)} \ .$$

If Y:negative hypergeometric(N, D, r) with

$$P(Y=y) = \begin{pmatrix} r+y-1 \\ y \end{pmatrix} \frac{(D)_r(N-D)_y}{(N)_{(r+y)}} \text{ for } y = 0, 1, \ldots, N-D,$$

then for the negative hypergeometric$(N+a+b-1, a+b-1, a)$ prior

$$P(D=d) = \begin{pmatrix} d+a-1 \\ d \end{pmatrix} \frac{(N)_d(a+b-1)_a}{(N+a+b-1)_{(a+d)}} \text{ for } d = 0, 1, \ldots, N$$

the posterior for $d = r, r+1, \ldots, N-y$ is

$$P(D = d|y) = \begin{pmatrix} d+a-1 \\ d-r \end{pmatrix} \frac{(N-r-y)_{d-r}(a+b+r+y-1)_{a+r}}{(N+a+b-1)_{(a+d)}} .$$

This is a negative hypergeometric$(N+a+b-1, a+b+r+y-1, a+r)$ distribution for D-r. For squarred error loss, the Bayes estimator is then

$$\hat{D}_B(y) = E(D|y) = r + \frac{(a+r)(N-r-y)}{(a+b+r+y)} .$$

11.8 Minimax Estimation

This approach to point estimation desires to minimize the maximum risk. Thus a minimax estimator $\delta_M(\mathbf{X})$ of $g(\theta)$ satisfies

$$\sup_\theta R_{\delta_M}(\theta) \leq \sup_\theta R_\delta(\theta)$$

for all estimators $\delta(\mathbf{X})$ of $g(\theta)$.

This approach guards against the worst case value of θ. It is a game theory approach with the statistician and nature as adversaries. Thus the statistician assumes that nature is trying select the true value of θ to maximize the risk. The statistician's strategy is that of selecting the estimator $\delta_M(\mathbf{X})$ to minimize this maximum risk. It is a conservative approach and guarding against the worst case parameter may degrade the estimator's performance for other parameter values.

There are several approaches to finding the minimax estimator.

Theorem 11.14 *Let $\Lambda(\theta)$ be a prior distribution over the parameter space Θ such that its Bayes estimator $\delta_B(\mathbf{X})$ satisfies*

$$r_{\delta_B}(\Lambda) = \int_{\theta\in\Theta} R_{\delta_B}(\theta) d\Lambda(\theta) = \sup_\theta R_{\delta_B}(\theta)$$

Then
(i) $\delta_B = \delta_M$ is minimax.
(ii) If δ_B is the unique Bayes estimator for the prior $\Lambda(\theta)$, then it is the unique Minimax estimator.
(iii) The prior distribution $\Lambda(\theta)$ is **least favorable**.

A prior $\Lambda(\theta)$ is said to be *least favorable* if its Bayes risk is maximum

$$r_{\delta_B}(\Lambda) \geq r_{\delta'_B}(\Lambda')$$

for all prior distributions $\Lambda'(\theta)$.
Proof.
(i) Let δ be any estimator. Then

$$\sup_\theta R_\delta(\theta) \geq \int_{\theta\in\Theta} R_\delta(\theta) d\Lambda(\theta) \geq \int_{\theta\in\Theta} R_{\delta_B}(\theta) d\Lambda(\theta) = \sup_\theta R_{\delta_B}(\theta) \ .$$

(ii) If δ_B is the unique Bayes estimator, then, if δ is any other estimator,

$$\sup_\theta R_\delta(\theta) \geq \int_{\theta\in\Theta} R_\delta(\theta) d\Lambda(\theta) > \int_{\theta\in\Theta} R_{\delta_B}(\theta) d\Lambda(\theta) = \sup_\theta R_{\delta_B}(\theta) \ .$$

(iii) Let $\Lambda'(\theta)$ be any other prior. Then

$$r_{\delta'_B}(\Lambda') = \int_{\theta\in\Theta} R_{\delta'_B}(\theta) d\Lambda'(\theta) \leq \int_{\theta\in\Theta} R_{\delta_B}(\theta) d\Lambda'(\theta) \leq \sup_\theta R_{\delta_B}(\theta) = r_{\delta_B}(\Lambda) \ . \blacksquare$$

Corollary 11.1 *If a Bayes estimator $\delta_B(\mathbf{X})$ has constant risk, then it is minimax.*

Proof.
If $R_{\delta_B}(\theta) = C$ then theorem (11.14) holds since

$$r_{\delta_B}(\Lambda) = \int_{\theta\in\Theta} C d\Lambda(\theta) = C = \sup_\theta C = \sup_\theta R_{\delta_B}(\theta) \ . \blacksquare$$

For an example of the use of the corollary, consider X:binomial(n, p). The bayes estimator (11.6) has risk

$$R_{\delta_B}(p) = E\left(\frac{(\alpha + X)}{(n + \alpha + \beta)} - p\right)^2 = \frac{npq}{(n + \alpha + \beta)^2} + \left(\frac{(\alpha + np)}{(n + \alpha + \beta)} - p\right)^2 \ .$$

When $\alpha = \beta = \sqrt{n}/2$ this risk is constant and equals

$$\frac{1}{4n(1 + 1/\sqrt{n})}$$

and the minimax estimator is

$$\hat{p}_M(x) = \frac{x + \sqrt{n}/2}{n + \sqrt{n}} \ .$$

Note the U.M.V.U. estimator $\hat{p}(x) = x/n$ has risk $p(1-p)/n$ and

$$\sup_p \frac{p(1-p)}{n} = \frac{1}{4n} > \frac{1}{4n(1 + 1/\sqrt{n})} \ .$$

However,

$$\frac{p(1-p)}{n} < \frac{1}{4n(1 + 1/\sqrt{n})}$$

for

$$p \notin \left(\frac{1 - \sqrt{1 - (1 + 1/\sqrt{n})^{-2}}}{2}, \frac{1 + \sqrt{1 - (1 + 1/\sqrt{n})^{-2}}}{2} \right)$$

which is all but a small interval about 1/2. The minimax estimator guards against the worst case parameter $p = 1/2$ at the expense of parameters outside of a small interval about 1/2.

Another example is X:hypergeometric(N, D, n) where D is the parameter, N, n known, and the loss is squarred error for estimating D. Then the estimator $\hat{D}(x) = \alpha x + \beta$ has risk

$$R_{\hat{D}}(D) = \alpha^2 \frac{nD(N-D)(N-n)}{N^2(N-1)} + \left(\frac{\alpha n D}{N} + \beta - D \right)^2 \ .$$

This is a constant β^2 when

$$\alpha = \frac{N}{n(1 + \sqrt{\frac{N-n}{n(N-1)}})}, \quad \beta = \frac{N\sqrt{\frac{N-n}{n(N-1)}}}{2(1 + \sqrt{\frac{N-n}{n(N-1)}})} \ .$$

This corresponds to the Bayes estimator for the prior (11.7) with

$$a = \frac{\beta}{\alpha - 1}, \quad b = \frac{N - n\alpha - \beta}{\alpha - 1} \ .$$

Thus

$$\hat{D}_M(x) = \frac{N}{n(1 + \sqrt{\frac{N-n}{n(N-1)}})} x + \frac{N}{n(1 + \sqrt{\frac{N-n}{n(N-1)}})}$$

is minimax with risk

$$\left(\frac{N}{n}\right)^2 \frac{n\left(\frac{N-n}{N-1}\right)}{4\left(1+\sqrt{\frac{N-n}{n(N-1)}}\right)^2} .$$

The U.M.V.U. estimator $\hat{D}(x) = Nx/n$ has risk

$$R_{\hat{D}}(D) = \left(\frac{N}{n}\right)^2 \frac{nD(N-D)(N-n)}{N^2(N-1)}$$

with maximum value

$$\sup_D R_{\hat{D}}(D) = \left(\frac{N}{n}\right)^2 \frac{n(N-n)}{4(N-1)} > \left(\frac{N}{n}\right)^2 \frac{n\left(\frac{N-n}{N-1}\right)}{4\left(1+\sqrt{\frac{N-n}{n(N-1)}}\right)^2} = R_{\hat{D}_M}(D) .$$

Although the maximum risk is larger that that for the minimax estimator, the risk of $\hat{D}(x)$ is smaller than that for $\hat{D}_M(x)$ when D is outside of a relatively small interval about $N/2$.

Another approach to finding minimax estimators uses the following theorem:

Theorem 11.15 *Let $\Lambda_m(\theta)$ be a sequence of priors with Bayes risk*

$$r_{\delta_B}(\Lambda_m) \longrightarrow r$$

and δ is an estimator with

$$\sup_\theta R_\delta(\theta) = r .$$

Then δ is minimax and for every prior $\Lambda(\theta)$ we have

$$r_{\delta_B}(\Lambda) \leq r .$$

Proof.
If δ^* is any other estimator,

$$\sup_\theta R_{\delta^*}(\theta) \geq \int_{\theta\in\Theta} R_{\delta^*}(\theta) d\Lambda_m(\theta) \geq r_{\delta_B}(\Lambda_m) \longrightarrow r = \sup_\theta R_\delta(\theta) .$$

Finally, for $\Lambda(\theta)$ is any prior,

$$r_{\delta_B}(\Lambda) = \int_{\theta\in\Theta} R_{\delta_B}(\theta)d\Lambda(\theta) \le \int_{\theta\in\Theta} R_\delta(\theta)d\Lambda(\theta) \le \sup_\theta R_\delta(\theta) = r \ . \blacksquare$$

For an example, let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ where $X_i : \mathcal{N}(\theta, \sigma^2)$ with σ^2 known. Consider the prior distribution $\Lambda(\theta)$ where $\theta : \mathcal{N}(\mu, m^2)$ with μ,m known. Then the Bayes estimator is

$$\delta_B(\mathbf{x}) = \frac{n\bar{x}/\sigma^2 + \mu/m^2}{n/\sigma^2 + 1/m^2} \ .$$

As $m \to \infty$, the Bayes risk

$$r_{\delta_B}(\Lambda) = \frac{1}{(n/\sigma^2 + 1/m^2)} \to r = \sigma^2/n \ .$$

Thus $\delta(\mathbf{x}) = \bar{x}$ has

$$R_\delta(\theta) = \frac{\sigma^2}{n} = r$$

and is minimax.

11.9 Problems

1. Let $X_1, X_2, \ldots, X_n$ be independent with density

$$f_{X_i}(x_i|\theta) = \frac{1}{(\theta_2 - \theta_1)} \text{ for } \theta_1 \le x_i \le \theta_2$$

where $\theta = (\theta_1, \theta_2)$. Derive the U.M.V.U. estimators for θ_1 and for θ_2.

2. Let $\mathbf{X}_i$ be independent $\mathcal{N}_p(\mu, \Sigma)$ for $i = 1, 2, \ldots, n$ where

$$\mu = (\mu_1, \mu_2, \ldots, \mu_p)^T \text{ and } \Sigma = (\sigma_{jk} : j, k = 1, 2, \ldots, p) \ .$$

Derive the U.M.V.U. estimators for μ_j and σ_{jk} for $1 \le j \le k \le p$.

3. Let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ have joint distribution

$$f_{\mathbf{X}}(\mathbf{x}|M) = \frac{1}{(M)_n} \text{ for } 0 \le x_i \le M$$

with integer x_i all different for $i = 1, 2, \ldots, n$. Derive the U.M.V.U. estimator for the integer parameter M.

4. If X:Poisson(θ). Show that the U.M.V.U. estimator for θ attains the Cramer-Rao-Frechet information lower bound for unbiased estimation.

5. Let $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_K)$ have joint distribution

$$P(\mathbf{Y} = \mathbf{y}) = \frac{(r + y_1 + y_2 + \cdots + y_K - 1)!}{(r-1)!y_1!y_2!\cdots y_K!} p_0^r p_1^{y_1} p_2^{y_2} \cdots p_K^{y_K}$$

$y_i = 0, 1, 2, \ldots, \infty, \quad i = 1, 2, \ldots, K$ where $p_0 + p_1 + p_2 + \cdots + p_K = 1$ and $0 < p_i < 1$. Derive the maximum likelihood estimators for p_i for $i = 1, 2, \ldots, K$. Prove that as $r \to \infty$,

$$\sqrt{r} \begin{pmatrix} \hat{p}_1 - p_1 \\ \hat{p}_2 - p_2 \\ \vdots \\ \hat{p}_K - p_K \end{pmatrix} \xrightarrow{d} \mathcal{N}_K(\mathbf{0}, \Sigma)$$

and give Σ.

6. Let X have a hypergeometric(N, D, n) distribution where N, n are known. Derive the maximum likelihood estimator for D and give its mean square error.

7. Let $\mathbf{X} = (X_1, X_2, \ldots, X_K)$ where

$$P(\mathbf{X} = \mathbf{x}) = \frac{n!}{x_1!x_2!\cdots x_K!} p_1^{x_1} p_2^{x_2} \cdots p_K^{x_K}$$

where $x_1 + x_2 + \cdots + x_K = n$ and

$$p_j = \binom{K}{j} p^j (1-p)^{K-j} \text{ for } 0 < p < 1 \ .$$

Derive the maximum likelihood estimator for p and give its exact distribution. Show that as $n \to \infty$ we have

$$\sqrt{n}(\hat{p} - p) \xrightarrow{d} \mathcal{N}(0, \sigma^2)$$

and give σ^2.

8. Let $X_1, X_2, \ldots, X_n$ be independent with

$$P(X_i = x_i | \theta) = \binom{r + (x_i - \nu) - 1}{r - 1} p^r (1-p)^{x_i - \nu}$$

for $x_i = \nu, \nu{+}1, \ldots, \infty$, $\theta = (p, \nu)$, $0 < p < 1$, $\nu \in \{0, \pm 1, \pm 2, \ldots, \pm\infty\}$. Derive the U.M.V.U. estimators for p and ν. Also derive the maximum likelihood estimators for p and ν.

9. Let $X_1, X_2, \ldots, X_n$ be independent $\mathcal{N}(-\sigma^2/2, \sigma^2)$. Derive the maximum likelihood estimator for σ^2. Show $\sqrt{n}(\hat{\sigma}^2 - \sigma^2) \xrightarrow{d} \mathcal{N}(0, \tau^2)$ and show $\tau^2 < 2\sigma^4$. Note for $S^2 = \sum_{i=1}^n (X_i - \bar{X})^2/(n-1)$ we have

$$\sqrt{n}(S^2 - \sigma^2)) \xrightarrow{d} \mathcal{N}(0, 2\sigma^4) \ .$$

10. Let $X_i, X_2, \ldots, X_n$ be independent with

$$f_{X_i}(x_i|\theta) = \frac{\alpha x_i^{-\alpha+1}}{\theta^\alpha} \text{ for } x_i > \theta, \ \ 0 \text{ elsewhere}$$

and $\alpha > 0$ known. For the prior density

$$\lambda(\theta) = \frac{(m-1)}{\theta^m} \text{ for } 1 < \theta < \infty, \text{ and } 0 \text{ elsewhere,}$$

give the Bayes estimator of θ using squarred error loss.

11. Let $X_1, X_2, \ldots, X_m$ be independent with continuous uniform density $R(0, \theta_1)$ and $Y_1, Y_2, \ldots, Y_n$ independent $R(0, \theta_2)$. Derive the U.M.V.U. estimator for $\rho = \theta_1/\theta_2$ and compare the mean square error with that of the maximum likelihood estimator $\hat{\rho}$.

12. Let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ have joint distribution for sampling without replacement given by

$$P(\mathbf{X} = \mathbf{x}) = \frac{1}{(M)_n} \text{ for all different } x_i \in \{1, 2, \ldots, M\}$$

$i = 1, 2, \ldots, n$, and $(M)_n = M(M-1)\cdots(M-n+1)$. Derive the U.M.V.U. estimator for M.

13. Let $\mathbf{X} = (X_1, X_2, \ldots, X_{K-1})$ have joint discrete distribution

$$P(\mathbf{X} = \mathbf{x}) = \frac{n!}{x_1! x_2! \cdots x_K!} p_1^{x_1} p_2^{x_2} \cdots p_K^{x_K}$$

where $\sum_{i=1}^K p_i = 1$, $0 < p_i < 1$, $\sum_{i=1}^K x_i = n$, and integer $x_i \in \{0, 1, \ldots, n\}$. Give the class of conjugate prior densities $\lambda(p_1, p_2, \ldots, p_{K-1})$ and give the corresponding Bayes estimator for $\sum_{i=1}^K a_i p_i$, where a_i are known, using squarred error loss.

14. Let X:Poisson(θ). Derive the minimax estimator for θ using loss function

$$L(\delta(x), \theta) = \frac{(\delta(x) - \theta)^2}{\theta} \ .$$

15. Let $X_1, X_2, \ldots, X_n$ be independent $\mathcal{N}(0, \sigma^2)$ Using loss

$$L(\delta(x), \sigma^2) = \left(\frac{\delta(x) - \sigma^2}{\sigma^2} \right)^2$$

derive the minimax estimator for σ^2.

Chapter 12

Hypothesis Testing

We next consider the hypothesis testing problem for observations $\mathbf{X}$ with distribution $P_\theta(\mathbf{x})$, $\theta \in \Theta$ of deciding between the hypothesis $\theta \in \Theta_H$ or the alternative hypothesis $\theta \in \Theta_A$ where $\Theta = \Theta_H \cup \Theta_A$. Neyman and Pearson considered error probabilities for a possibly randomized decision rule. Let $\phi(\mathbf{x})$ be the probability of deciding $\theta \in \Theta_A$ given $\mathbf{x}$. Then the type I error probability

$$\alpha = \sup_{\theta \in \Theta_H} E_\theta(\phi(\mathbf{X}))$$

and the type II error probabilities

$$\beta(\theta) = E_\theta(1 - \phi(\mathbf{X})) \text{ for } \theta \in \Theta_A \ .$$

Because one type of error may be of more concern than the other, the *null* hypothesis Θ_H is labeled so that the type I error is the more serious with the type II error for the *alternative* hypothesis Θ_A the less serious. Then the Neyman-Pearson formulation puts a bound on the type I error probability α and subject to this bound, tries to select a decision rule to minimize the type II error probabilities $\beta(\theta)$ for $\theta \in \Theta_A$.

The *power function* of a test ϕ is defined by

$$\gamma(\theta) = E_\theta(\phi(\mathbf{X})) \text{ for } \theta \in \Theta \ .$$

Then the type I error

$$\alpha = \sup_{\theta \in \Theta_H} \gamma(\theta)$$

and the type II error

$$\beta(\theta) = 1 - \gamma(\theta) \text{ for } \theta \in \Theta_A \ .$$

12.1 Simple Hypotheses

For the case where $\Theta_H = \{\theta_0\}$ and $\Theta_A = \{\theta_1\}$ each have just one element (simple null hypothesis and simple alternative hypothesis) the Neyman - Pearson fundamental lemma gives a solution for the best decision rule based on the likelihood ratio statistic

$$L(\mathbf{x}) = \frac{f(\mathbf{x}|\theta_1)}{f(\mathbf{x}|\theta_0)}$$

where $f(\mathbf{x}|\theta)$ is the density of $P_\theta(\mathbf{x})$ with respect to a measure $\mu(\mathbf{x})$. Note, since P_{θ_0} and $P_{\theta_1} << P_{\theta_0} + P_{\theta_1}$ such densities exist by the Radon-Nikodym theorem.

Lemma 12.1 Neyman-Pearson fundamental lemma.
(i) For testing the simple null hypothesis against the simple alternative hypothesis

$$H : \theta = \theta_0 \text{ vs. } A : \theta = \theta_1$$

the decision rule

$$\phi(\mathbf{x}) = \begin{cases} 1 & \text{for } L(\mathbf{x}) > C \\ \xi & \text{for } L(\mathbf{x}) = C \\ 0 & \text{for } L(\mathbf{x}) < C \end{cases} \tag{12.1}$$

where C, ξ are determined so that

$$E_{\theta_0}(\phi(\mathbf{X})) = \alpha \tag{12.2}$$

minimizes the type two error $\beta(\theta_1)$ (is most powerful).
(ii) If a test with type I error α has smallest type II error for testing θ_0 vs. θ_1 then it satisfies

$$\phi(\mathbf{x}) = \begin{cases} 1 & \text{for } L(\mathbf{x}) > C \\ 0 & \text{for } L(\mathbf{x}) < C \end{cases}$$

unless there exists a test with $E_{\theta_0}(\phi(\mathbf{X})) < \alpha$ and $\beta(\theta_1) = 0$.

Proof.
(i) For $\alpha = 0$ take $C = \infty$. For $\alpha = 1$ take $C = -\infty$.
Next assume $0 < \alpha < 1$ and define

$$\alpha(C) = P_{\theta_0}(f(\mathbf{X}|\theta_1) > Cf(\mathbf{X}|\theta_0)) \ .$$

Then $1-\alpha(C)$ is the c.d.f. for $L(\mathbf{X})$ and

$$(1-\alpha(C))-(1-\alpha(C-0)) = P_{\theta_0}(L(\mathbf{X})=C),$$

$\alpha(-\infty)=1$, $\alpha(\infty)=0$, and $\alpha(C)\downarrow$. Let C_0 satisfy $\alpha(C_0)\le\alpha\le\alpha(C_0-0)$ and define

$$\phi(\mathbf{x}) = \begin{cases} 1 & \text{for } L(\mathbf{x})>C_0 \\ \xi_0 & \text{for } L(\mathbf{x})=C_0 \\ 0 & \text{for } L(\mathbf{x})<C_0 \end{cases} \quad \text{where } \xi_0 = \frac{\alpha-\alpha(C_0)}{\alpha(C_0-0)-\alpha(C_0)}\ .$$

If $\alpha(C_0)=\alpha(C_0-0)$ take $\xi_0=0$. Then

$$E_{\theta_0}(\phi(\mathbf{X})) = 1P(L(\mathbf{X})>C_0)+\xi_0 P(L(\mathbf{X})=C_0)$$

$$= \alpha(C_0)+\left(\frac{\alpha-\alpha(C_0)}{\alpha(C_0-0)-\alpha(C_0)}\right)(\alpha(C_0-0)-\alpha(C_0)) = \alpha$$

and $C=C_0\ge 0$ satisfies (12.1) and (12.2).
(ii) Now let $\phi^*(\mathbf{x})$ be any other decision rule with type I error $\alpha^*\le\alpha$ and define

$$\mathcal{S}^+ = \{\mathbf{x}:\phi(\mathbf{x})-\phi^*(\mathbf{x})>0\} \text{ and } \mathcal{S}^- = \{\mathbf{x}:\phi(\mathbf{x})-\phi^*(\mathbf{x})<0\}\ .$$

Then

$$\int_{\mathbf{x}\in\mathcal{X}} (\phi(\mathbf{x})-\phi^*(\mathbf{x}))(f(\mathbf{x}|\theta_1)-C_0 f(\mathbf{x}|\theta_0))d\mu(\mathbf{x})$$

$$= \int_{\mathbf{x}\in\mathcal{S}^+\cup\mathcal{S}^-} (\phi(\mathbf{x})-\phi^*(\mathbf{x}))(f(\mathbf{x}|\theta_1)-C_0 f(\mathbf{x}|\theta_0))d\mu(\mathbf{x}) \ge 0$$

since for $\mathbf{x}\in\mathcal{S}^+$, $\phi(\mathbf{x})>0$ and $f(\mathbf{x}|\theta_1)-C_0 f(\mathbf{x}|\theta_0)\ge 0$, for $\mathbf{x}\in\mathcal{S}^-$, $\phi(\mathbf{x})<1$ and $f(\mathbf{x}|\theta_1)-C_0 f(\mathbf{x}|\theta_0)\le 0$. Thus in both cases the the integrand product is non negative and

$$\int_{\mathbf{x}\in\mathcal{X}} (\phi(\mathbf{x})-\phi^*(\mathbf{x}))f(\mathbf{x}|\theta_1)d\mu(\mathbf{x})$$

$$\ge \int_{\mathbf{x}\in\mathcal{X}} (\phi(\mathbf{x})-\phi^*(\mathbf{x}))C_0 f(\mathbf{x}|\theta_0)d\mu(\mathbf{x}) = C_0(\alpha-\alpha^*)\ge 0\ .$$

(ii) Let $\phi^*(\mathbf{x})$ be a type I error α test with smallest type II error $\beta^*$and define

$$\mathcal{S} = \{\mathbf{x}: f(\mathbf{x}|\theta_1)\ne C_0 f(\mathbf{x}|\theta_0)\}\cap(\mathcal{S}^+\cup\mathcal{S}^-)\ .$$

Then

$$(\phi(\mathbf{x}) - \phi^*(\mathbf{x}))(f(\mathbf{x}|\theta_1) - C_0 f(\mathbf{x}|\theta_0)) > 0 \text{ for } \mathbf{x} \in \mathcal{S}$$

and if $\mu(\mathcal{S}) > 0$ then

$$\int_{\mathbf{x}\in\mathcal{S}^+\cup\mathcal{S}^-} (\phi(\mathbf{x}) - \phi^*(\mathbf{x}))(f(\mathbf{x}|\theta_1) - C_0 f(\mathbf{x}|\theta_0)) d\mu(\mathbf{x})$$

$$= \int_{\mathbf{x}\in\mathcal{S}} (\phi(\mathbf{x}) - \phi^*(\mathbf{x}))(f(\mathbf{x}|\theta_1) - C_0 f(\mathbf{x}|\theta_0)) d\mu(\mathbf{x}) > 0 \ .$$

Thus for ϕ we have $1-\beta \geq 1-\beta^*$ for ϕ^* which is a contradiction and $\mu(\mathcal{S}) = 0$. If ϕ^* has type I error $< \alpha$ then we can add points $\mathbf{x}$ to the rejection region (increase $\phi(\mathbf{x})$) until either $E_{\theta_0}(\phi(\mathbf{X})) = \alpha$ or $E_{\theta_1}(\phi(\mathbf{X})) = 1 - \beta^* = 1$. ■

12.2 Composite Hypotheses

12.2.1 Distributions with Monotone Likelihood Ratio

We say the distribution $f(\mathbf{x}|\theta)$ has monotone likelihood ratio if there exists a statistic $T(\mathbf{x})$ such that

$$\frac{f(\mathbf{x}|\theta_1)}{f(\mathbf{x}|\theta_0)} \text{ for all } \theta_0 < \theta_1$$

is increasing in $T(\mathbf{x})$.

For example if $X_1, X_2, \ldots, X_n$ are independent $\mathcal{N}(0, \sigma^2)$ then for $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ we have

$$f(\mathbf{x}|\sigma^2) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^n \exp\{-\frac{1}{2\sigma^2}\sum_{i=1}^n x_i^2\}$$

has monotone likelihood ratio with $T(\mathbf{x}) = \sum_{i=1}^n x_i^2$.

12.2.2 U.M.P. One Sided Tests

Theorem 12.1 *For testing composite one sided hypotheses*

$$H\text{: } \theta \leq \theta_0 \ \textit{vs.} \ A\text{: } \theta > \theta_0$$

for distributions with monotone likelikood ratio there exists a uniformly most powerful (U.M.P.) test given by

$$\phi(\mathbf{x}) = \begin{cases} 1 & \textit{for } T(\mathbf{x}) > C \\ \xi & \textit{for } T(\mathbf{x}) = C \\ 0 & \textit{for } T(\mathbf{x}) < C \end{cases} \quad \textit{where } C, \xi \textit{ satisfy } E_{\theta_0}(\phi(\mathbf{X})) = \alpha \ .$$

Proof.
We consider the most powerful test of the simple H: $\theta = \theta_0$ vs. simple A: $\theta = \theta_1$ where $\theta_1 > \theta_0$. Then using the Neyman-Pearson fundamental lemma, the most powerful likelihood ratio test is

$$\phi(\mathbf{x}) = \begin{cases} 1 & \text{for } L(\mathbf{x}) > C_0 \\ \xi_0 & \text{for } L(\mathbf{x}) = C_0 \\ 0 & \text{for } L(\mathbf{x}) < C_0 \end{cases} \quad \text{where } C_0, \xi_0 \text{ satisfy } E_{\theta_0}(\phi(\mathbf{X})) = \alpha \ .$$

Using the monotone likelihood ratio property, this (for appropriate C, ξ) is equivalent to

$$\phi(\mathbf{x}) = \begin{cases} 1 & \text{for } T(\mathbf{x}) > C \\ \xi & \text{for } T(\mathbf{x}) = C \\ 0 & \text{for } T(\mathbf{x}) < C \end{cases} \quad \text{where } C, \xi \text{ satisfy } E_{\theta_0}(\phi(\mathbf{X})) = \alpha \ . \tag{12.3}$$

Next we show the power function of the test $\gamma(\theta)$ is strictly increasing in θ for all $\gamma(\theta) > 0$ so that $\gamma(\theta) \le \alpha$ for $\theta \le \theta_0$ and the test has type I error α. Consider $\theta' < \theta''$ and let $\alpha' = E_{\theta'}(\phi(\mathbf{X}))$. Then ϕ is most powerful for testing θ' vs. θ'' and considering the trivial test $\phi^* \equiv \alpha'$ which has power $E_{\theta''}(\phi^*(\mathbf{X})) = \alpha' \le E_{\theta''}(\phi(\mathbf{X}))$ since ϕ is most powerful.
Finally, since the test ϕ of type I error α for H is most powerful against θ_1 and does not depend on the choice of θ_1, it is uniformly most powerful. ∎

If $F_T(t)$ is the c.d.f., then the condition that C, ξ satisfy $E_{\theta_0}(\phi(\mathbf{X})) = \alpha$ is equivalent to

$$F_T(C-) \le 1 - \alpha, \quad F_T(C) > 1 - \alpha$$

$$\xi = \frac{F_T(C) - (1-\alpha)}{F_T(C) - F_T(C-)} \ . \tag{12.4}$$

As an example, let X have a binomial(n, p) distribution and consider H: $p \le p_0$ vs. A: $p > p_0$. Then, since the binomial distribution has a monotone likelihood ratio with $T(x) = x$, the U.M.P. test is given by (12.3) and

(12.4) where, expressing the binomial c.d.f. in terms of the incomplete beta function,

$$F_X(C) = \sum_{x=0}^{C} \binom{n}{x} p_0^x (1-p_0)^{n-x} = I_{(1-p_0)}(n-C, C+1), \; F_X(C-) = F_X(C-1).$$

For another example, if X: hypergeometric(N, D, n) testing H: $D \le D_0$ vs. A: $D > D_0$, the U.M.P. test is given by (12.3) and (12.4) with $T(x) = x$ and for $L = \max(0, n + D_0 - N)$,

$$F_X(C) = F_X(C; N, D_0, n) = \sum_{x=L}^{C} \binom{n}{x} \binom{N-n}{D_0-x} \Big/ \binom{N}{D_0},$$

$$F_X(C-) = F_X(C-1) \; .$$

If X: Poisson(λ), the U.M.P. test of H: $\lambda \le \lambda_0$ vs. A: $\lambda > \lambda_0$ is given by (12.3) and (12.4) with $T(x) = x$ where the Poisson c.d.f. expressed in terms of the incomplete gamma function is

$$F_X(C) = \sum_{x=0}^{C} \frac{\lambda_0^x}{x!} e^{-\lambda_0} = 1 - G(\lambda_0, C+1), \quad F_X(C-) = F_X(C-1) \; .$$

If X: negative binomial(r, p) testing H: $p \le p_0$ vs. A: $p > p_0$, then we have monotone likelihood ratio with $T(x) = -x$ and the U.M.P. test is

$$\phi(x) = \begin{cases} 1 & \text{if } x < C \\ \xi & \text{if } x = C \\ 0 & \text{if } x > C \end{cases}$$

where C, ξ satisfy

$$F_X(C) = \sum_{x=0}^{C} \binom{r+x-1}{x} p_0^r (1-p_0)^x = I_{p_0}(r, C+1) > \alpha, \quad F_X(C-1) \le \alpha,$$

$$\xi = \frac{\alpha - F_X(C-1)}{F_X(C) - F_X(C-1)} \; .$$

The C++ program **Test.cpp** in **Appendix D** calculates C, ξ given α and the parameters for these examples.

12.2.3 P-Values

For a test that rejects the hypothesis for large values of a statistic ($T(\mathbf{X}) \geq C_\alpha$) a convenient decision rule is one using the P-value

$$\hat{\alpha}(t) = P_H(T(\mathbf{X}) \geq t)$$

where t is the observed value of $T(\mathbf{X})$. Then if we reject if

$$\alpha \geq \hat{\alpha}(t)$$

it is equivalent to rejecting if $t = T(\mathbf{x}) \geq C_\alpha$ where $\alpha = P_H(T(\mathbf{X}) \geq C_\alpha)$. The P-value is the smallest value of α for which we can reject the hypothesis for the given value of the data $t = T(\mathbf{x})$.

To illustrate, let $X_1, X_2, \ldots, X_n$ be independent $\mathcal{N}(0, \sigma^2)$. For testing H: $\sigma^2 \leq 2.5$ vs. A: $\sigma^2 > 2.5$ the U.M.P. test rejects if

$$\sum_{i=1}^{n} X_i^2/2 \geq \chi^2_{n,\alpha}$$

where $P(\chi^2_n \geq \chi^2_{n,\alpha}) = \alpha$. For a sample of size $n = 12$ with $\sum_{i=1}^{12} X_i^2 = 53.7$, the P-value, using the incomplete gamma for the chi square distribution, is

$$\hat{\alpha} = P(\chi^2_{12} \geq 53.7/2.5) = 1 - G(53.7/(2 \times 2.5), 12/2) = 0.0437782$$

and we can reject using type I error α for any $\alpha \geq \hat{\alpha} = 0.0437782$.

12.2.4 Least Favorable Priors

Another method to derive a most powerful test of a composite hypothesis versus a simple alternative uses a *least favorable prior* over the parameters in the composite null hypothesis when such exist.

Definition 12.1 *Let the composite null hypothesis H: $\theta \in \Theta_H$ have a prior distribution $\Lambda(\theta)$ for $\theta \in \Theta_H$. Then if $\mathbf{X}$ has density $f(\mathbf{x}|\theta)$, define*

$$g_\Lambda(\mathbf{x}) = \int_{\theta \in \Theta_H} f(\mathbf{x}|\theta) d\Lambda(\theta) \ . \tag{12.5}$$

We say $\Lambda(\theta)$ is **least favorable** *if, for the simple alternative $h(\mathbf{x})$, the maximum power β_Λ for testing $g_\Lambda(\mathbf{x})$ vs. $h(\mathbf{x})$ satisfies $\beta_\Lambda \leq \beta_{\Lambda'}$ for any other prior $\Lambda'(\theta)$, $\theta \in \Theta_H$. Here $\beta_{\Lambda'}$ is the maximum power for testing $g_{\Lambda'}(\mathbf{x})$ vs. $h(\mathbf{x})$.*

We then have the following

Theorem 12.2 *If $\phi_\Lambda(\mathbf{x})$ is most powerful for testing H_Λ: $g_\Lambda(\mathbf{x})$ vs. A: $h(\mathbf{x})$, where $g_\Lambda(\mathbf{x})$ is given by (12.5), and has type I error α for H: $f(\mathbf{x}|\theta), \theta \in \Theta_H$, then it is most powerful for testing H vs. A and Λ is least favorable.*

Proof.
Let $\phi^*(\mathbf{x})$ be a test of H vs. A with type I error $E_\theta(\phi^*(\mathbf{X})) \leq \alpha$ for $\theta \in \Theta_H$. Then, interchanging the order of integration,

$$\int_{\mathbf{x}\in\mathcal{X}} \phi^*(\mathbf{x}) g_\Lambda(\mathbf{x}) d\mu(\mathbf{x}) = \int_{\theta\in\Theta_H} E_\theta(\phi^*(\mathbf{X})) d\Lambda(\theta) \leq \alpha$$

and $\phi^*(\mathbf{x})$ is a test with type I error at most α for testing H_Λ vs. A. Thus $\phi(\mathbf{x})$ is at least as powerful as $\phi^*(\mathbf{x})$. Next, if $\Lambda'(\theta)$ is any other prior on Θ_H, then $\phi_\Lambda(\mathbf{x})$ has type I error α for testing $\mathrm{H}_{\Lambda'}$ vs. A. Thus $\beta_\Lambda \leq \beta_{\Lambda'}$ since the power of $\phi(\mathbf{x})$ cannot exceed the power of the most powerful test of $\mathrm{H}_{\Lambda'}$ vs. A. ∎

We use the Neyman-Pearson fundamental lemma to derive the most powerful test of $g_\Lambda(\mathbf{x})$ vs $h(\mathbf{x})$ based on the likelihood ratio for an appropriate least favorable prior $\Lambda(\theta)$.

For an example, let $X_1, X_2, \ldots, X_n$ be independent $\mathcal{N}(\mu, \sigma^2)$ where $\theta = (\mu, \sigma^2)$. To derive the U.M.P. test of H: $\sigma^2 \leq \sigma_0^2$, $-\infty < \mu < \infty$ vs. A: $\sigma^2 > \sigma_0^2$, $-\infty < \mu < \infty$, consider the simple alternative (μ_1, σ_1^2) where $\sigma_0^2 < \sigma_1^2$. Reducing the problem by sufficiency, we have $(\bar{X}, S^2)$ is sufficient for $\theta = (\mu, \sigma^2)$ where

$$\bar{X} = \sum_{i=1}^n X_i/n, \quad S^2 = \sum_{i=1}^n (X_1 - \bar{X})^2/(n-1) \ .$$

which are independent $\mathcal{N}(\mu, \sigma^2/n)$ and $(\sigma^2/(n-1))\chi^2_{(n-1)}(0)$ respectively. If we consider the prior $\Lambda(\theta)$ that puts probability 1 on the line $\sigma^2 = \sigma_0^2$ and $\mu : \mathcal{N}(\mu_1, (\sigma_1^2 - \sigma_0^2)/n)$ then forming the convolution of a $\mathcal{N}(0, \sigma_0^2/n)$ and a $\mathcal{N}(\mu_1, (\sigma_1^2 - \sigma_0^2)/n)$ random variable gives a $\mathcal{N}(\mu_1, \sigma_1^2/n)$ result and

$$g_\Lambda(\bar{x}, s^2) = \frac{(s^2)^{(n-1)/2-1} e^{-(n-1)s^2/(2\sigma_0^2)}}{\Gamma((n-1)/2) 2^{(n-1)/2} (\sigma_0^2/(n-1))^{(n-1)/2}} \frac{\sqrt{n}}{\sigma_1\sqrt{2\pi}} e^{-n(\bar{x}-\mu_1)^2/(2\sigma_1^2)} \ .$$

The likelihood ratio test then rejects for large values of

$$\frac{h(\bar{X}, S^2)}{g_\Lambda(\bar{X}, S^2)} = \left(\frac{\sigma_1}{\sigma_0}\right)^{n-1} e^{(n-1)S^2(1/(2\sigma_0^2) - 1/(2\sigma_1^2))}$$

which is equivalent to rejecting if

$$\frac{(n-1)S^2}{\sigma_0^2} \geq \chi^2_{n-1,\alpha} \ .$$

Since this test has type I error α for H and does not depend on μ_1 and σ_1^2, it is U.M.P. for H vs. A.

12.2.5 U.M.P.Unbiased Tests

When no U.M.P. test exists, we can consider restricting attention to tests that are unbiased and then finding the uniformly most powerful test within this class.

Definition 12.2 *We say a test $\phi(\mathbf{x})$ is* **unbiased** *if*

$$E_\theta(\phi(\mathbf{X})) \leq \alpha \ for \ \theta \in \Theta_H, \quad E_\theta(\phi(\mathbf{X})) \geq \alpha \ for \ \theta \in \Theta_A \ .$$

If we denote the boundary $\omega = \bar{\Theta}_H \cap \bar{\Theta}_A$ (the intersection of the closures of Θ_H and Θ_A) then, if the power function of an unbiased test is continuous, we have $\beta(\theta) = E_\theta(\phi(\mathbf{X})) = \alpha$ for $\theta \in \omega$. The test is then said to be similar on the boundary ω.

For a one parameter exponential family with density

$$\frac{dP_\theta}{d\mu}(\mathbf{x} = C(\theta)e^{\theta T(\mathbf{x})}h(\mathbf{x})$$

the power function of a test $\phi(\mathbf{x})$ is continuous. For testing

(1) H_1: $\theta \leq \theta_0$ vs. A_1: $\theta > \theta_0$
(2) H_2: $\theta \leq \theta_1$ or $\theta \geq \theta_2$ vs. A_2: $\theta_1 < \theta < \theta_2$
(3) H_3: $\theta_1 \leq \theta \leq \theta_2$ vs. A_3: $\theta < \theta_1$ or $\theta > \theta_2$
(4) H_4: $\theta = \theta_0$ vs. A_4: $\theta \neq \theta_0$

there exists U.M.P. unbiased tests given by

$$\begin{aligned}
\phi_1(t) &= \begin{cases} 1 \text{ if } t > c_0 \\ \xi_1 \text{ if } t = c_0 \quad \text{where } E_{\theta_0}(\phi_1(T)) = \alpha \\ 0 \text{ if } t < c_0 \end{cases} \\
\phi_2(t) &= \begin{cases} 1 \text{ if } c_1 < t < c_2 \\ \xi_2 \text{ if } t = c_i \qquad \text{where } E_{\theta_i}(\phi_2(T)) = \alpha, \;\; i = 1,2 \\ 0 \text{ if } t < c_1 \text{ or } t > c_2 \end{cases} \\
\phi_3(t) &= \begin{cases} 1 \text{ if } t < c_1 \text{ or } t > c_2 \\ \xi_3 \text{ if } t = c_i \qquad \text{where } E_{\theta_i}(\phi_3(T)) = \alpha, \;\; i = 1,2 \\ 0 \text{ if } c_1 < t < c_2 \end{cases} \\
\phi_4(t) &= \begin{cases} 1 \text{ if } t < c_1 \text{ or } t > c_2 \\ \xi_4 \text{ if } t = c_i \quad i = 1,2 \\ 0 \text{ if } c_1 < t < c_2 \end{cases} \\
&\text{where } E_{\theta_0}(\phi_4(T)) = \alpha, \quad E_{\theta_0}(T\phi_4(T)) = \alpha E_{\theta_0}(T) \; .
\end{aligned}$$

Proofs are given by Lehmann[1] using the folowing extension of the Neyman-Pearson fundamental lemma.

Lemma 12.2 *Let $f_0, f_1, \ldots, f_m$ be real valued functions that are integrable with respect to a measure μ. Let ϕ be a critical function such that*

$$\int \phi(x) f_i(x) d\mu(x) = c_i \text{ for } i = 1, 2, \ldots, m. \tag{12.6}$$

If $\mathcal{C}$ is the class of critical functions satisfying (12.6) there exists a $\phi \in \mathcal{C}$ that maximizes

$$\int \phi(x) f_0(x) d\mu(x) \; .$$

A sufficient condition to maximize is the existance of constants $k_1, k_2, \ldots, k_m$ such that

$$\phi(x) = 1 \text{ if } f_0(x) > \sum_{i=1}^{m} k_i f_i(x)$$

$$\phi(x) = 0 \text{ if } f_0(x) < \sum_{i=1}^{m} k_i f_i(x) \; . \tag{12.7}$$

[1]E.L.Lehmann (1991),*Testing Statistical Hypotheses, Second Edition* Wadsworth & Brooks/Cole, Pages 135-137.

If $\phi \in \mathcal{C}$ satisfies (12.7) with $k_i \geq 0$ for $i = 1, 2, \ldots, m$ then it maximizes $\int \phi(x) f_0(x) d\mu(x)$ among all ϕ such that

$$\int \phi(x) f_i(x) d\mu(x) \leq c_i \text{ for } i = 1, 2, \ldots, m.$$

For an example, let X have a Poisson(θ) distribution and consider H: $\theta = \theta_0$ vs. A: $\theta \neq \theta_0$ then the U.M.P unbiased test is given by ϕ_4 with $T(x) = x$ and c_1, c_1, ξ_1, ξ_2 determined by

$$\sum_{x=c_1+1}^{c_2-1} \frac{\theta_0^x e^{-\theta_0}}{x!} + (1-\xi_1)\frac{\theta_0^{c_1} e^{-\theta_0}}{c_1!} + (1-\xi_2)\frac{\theta_0^{c_2} e^{-\theta_0}}{c_2!} = 1 - \alpha$$

$$\sum_{y=C_1}^{c_2-2} \frac{\theta_0^x e^{-\theta_0}}{x!} + (1-\xi_1)\frac{\theta_0^{c_1-1} e^{-\theta_0}}{(c_1-1)!} + (1-\xi_2)\frac{\theta_0^{c_2-1} e^{-\theta_0}}{(c_2-1)!} = 1 - \alpha\ .$$

This requires trial and error so that for

$$F_X(x) = \sum_{y=0}^{x} \frac{\theta_0^y e^{-\theta_0}}{y!}$$

we have c_1 and c_2 satisfy

$$F_X(c_2) - F_X(c_1 - 1) > 1 - \alpha, \quad F_X(c_2 - 1) - F_X(c_1) \leq 1 - \alpha$$

$$F_X(c_2 - 1) - F_X(c_1 - 2) > 1 - \alpha, \quad F_X(c_2 - 2) - F_X(c_1 - 1) \leq 1 - \alpha\ .$$

We then solve the following linear equations for $\xi_1,\ \xi_2$

$$(1-\xi_1)\frac{\theta_0^{c_1} e^{-\theta_0}}{(c_1)!} + (1-\xi_2)\frac{\theta_0^{c_2} e^{-\theta_0}}{(c_2)!} = (1-\alpha) - (F_X(c_2-1) - F_X(c_1))$$

$$(1-\xi_1)\frac{\theta_0^{c_1-1} e^{-\theta_0}}{(c_1-1)!} + (1-\xi_2)\frac{\theta_0^{c_2-1} e^{-\theta_0}}{(c_2-1)!} = (1-\alpha) - (F_X(c_2-2) - F_X(c_1-1)).$$

If the constraints $0 \leq \xi_1, \xi_2 \leq 1$ are not satisfied, then iteration continues on the choice of c_1, c_2 until they are.

Another important class of distributions for which the power function of a test is continuous is the exponential family with parameter θ and nuisance parameters $\nu = (\nu_1, \nu_2, \ldots, \nu_k)$ given by

$$\frac{dP_\theta}{d\mu}(\mathbf{x}) = C(\theta, \nu) \exp\{\theta u(\mathbf{x}) + \sum_{i=1}^{k} \nu_i t_i(\mathbf{x})\}\ . \tag{12.8}$$

For testing hypotheses and alternatives about θ, such as H: $\theta = \theta_0$, we have

$$\omega = \{(\theta_0, \nu) : \nu \in \Upsilon\}$$

where Υ is the natural parameter space of $dP_{\theta_0,\nu}/d\mu$. The sufficient statistic for ω is $\mathbf{T}(\mathbf{X}) = (t_1(\mathbf{X}), t_2(\mathbf{X}), \ldots, t_k(\mathbf{X}))$ and we can construct a similar test if

$$E(\phi(\mathbf{X})|\mathbf{T}(\mathbf{X}) = \mathbf{t}) = \alpha$$

since then

$$E_\omega(E(\phi(\mathbf{X})|\mathbf{T}(\mathbf{X})) = E_\omega(\alpha) = \alpha \ .$$

Such conditional tests are called tests of *Neyman structure*.

Theorem 12.3 *All similer tests to have Neyman structure if and only if ($\Longleftrightarrow$) the sufficient statistic $\mathbf{T}(\mathbf{X})$ for ω is boundedly complete.*

Proof.
($\Longleftarrow$) If $\mathbf{T}(\mathbf{X})$ is boundedly complete, let $\phi(\mathbf{X})$ be a similar test. Then

$$E_\omega(\phi(\mathbf{X}) - \alpha) = 0 \ .$$

Then for $\psi(\mathbf{t}) = E(\phi(\mathbf{X}) - \alpha|\mathbf{T}(\mathbf{X}) = \mathbf{t})$ we have

$$E_\omega(\psi(\mathbf{T})) = E_\omega(E(\phi(\mathbf{X}) - \alpha|\mathbf{T})) = E_\omega(\phi(\mathbf{X}) - \alpha) = 0 \ .$$

Since $\psi(\mathbf{t})$ is bounded, we have $\psi(\mathbf{t}) = 0$ by bounded completeness and we have Neyman structure since

$$E(\phi(\mathbf{X}) - \alpha|\mathbf{T}(\mathbf{X}) = \mathbf{t}) = 0 \ .$$

($\Longrightarrow$) Let all similar tests have Neyman structure and let $\psi(\mathbf{t})$ be bounded, $|\psi(\mathbf{t})| \leq K$, with

$$E_\omega(\psi(\mathbf{T})) = 0 \ .$$

Then $C\psi(\mathbf{t}) + \alpha$ where $C = \min\{\alpha, 1 - \alpha\}/K$ is a similar test since it is between 0 and 1 and

$$E_\omega(C\psi(\mathbf{T}) + \alpha) = 0 + \alpha \text{ for } \theta \in \omega \ .$$

Thus by the assumption, it has Neyman structure and

$$E(C\psi(\mathbf{T}(\mathbf{X})) + \alpha|\mathbf{T}(\mathbf{X}) = \mathbf{t}) = C\psi(\mathbf{t}) + \alpha = \alpha \ .$$

So $\psi(\mathbf{t}) = 0$ since $C > 0$ and we have bounded completeness. ■

Applying Neyman structure and the extension of the fundamental lemma to the exponential family with density with respect to a measure $\mu(\mathbf{x})$ given by (12.8) we have the following

Theorem 12.4 *For the exponential distribution (12.8) with parameter space containing a $k+1$ dimensional rectangle, testing*

$$\begin{array}{l}
(1)\ H_1\colon\ \theta \le \theta_0 \ \ vs.\ A_1\colon\ \theta > \theta_0 \\
(2)\ H_2\colon\ \theta \le \theta_1 \ \ or\ \theta \ge \theta_2 \ \ vs.\ A_2\colon\ \theta_1 < \theta < \theta_2 \\
(3)\ H_3\colon\ \theta_1 \le \theta \le \theta_2 \ \ vs.\ A_3\colon\ \theta < \theta_1 \ \ or\ \theta > \theta_2 \\
(4)\ H_4\colon\ \theta = \theta_0 \ \ vs.\ A_4\colon\ \theta \ne \theta_0
\end{array}$$

there exist uniformly most powerful unbiased tests given by

$$\phi_1(u,\mathbf{t}) = \begin{cases} 1 \ \ if\ u > c_0(\mathbf{t}) \\ \xi_1(\mathbf{t}) \ \ if\ u = c_0(\mathbf{t}) \quad where\ E_{\theta_0}(\phi_1(U,\mathbf{T})|\mathbf{T}=\mathbf{t}) = \alpha \\ 0 \ \ if\ u < c_0(\mathbf{t}) \end{cases}$$

$$\phi_2(u,\mathbf{t}) = \begin{cases} 1 \ \ if\ c_1(\mathbf{t}) < u < c_2(\mathbf{t}) \\ \xi_2(\mathbf{t}) \ \ if\ u = c_i(\mathbf{t}) \qquad where\ E_{\theta_i}(\phi_2(U,\mathbf{T})|\mathbf{T}=\mathbf{t}) = \alpha, \ \ i=1,2 \\ 0 \ \ if\ u < c_1(\mathbf{t}) \ \ or\ u > c_2(\mathbf{t}) \end{cases}$$

$$\phi_3(u,\mathbf{t}) = \begin{cases} 1 \ \ if\ u < c_1(\mathbf{t}) \ \ or\ u > c_2(\mathbf{t}) \\ \xi_3(\mathbf{t}) \ \ if\ u = c_i(\mathbf{t}) \qquad where\ E_{\theta_i}(\phi_3(U,\mathbf{T})|\mathbf{T}=\mathbf{t}) = \alpha, \ \ i=1,2 \\ 0 \ \ if\ c_1(\mathbf{t}) < u < c_2(\mathbf{t}) \end{cases}$$

$$\phi_4(u,\mathbf{t}) = \begin{cases} 1 \ \ if\ u < c_1(\mathbf{t}) \ \ or\ u > c_2(\mathbf{t}) \\ \xi_4(\mathbf{t}) \ \ if\ u = c_i(\mathbf{t}) \quad i=1,2 \\ 0 \ \ if\ c_1(\mathbf{t}) < u < c_2(\mathbf{t}) \end{cases}$$

$$where\ E_{\theta_0}(\phi_4(U,\mathbf{T})|\mathbf{T}=\mathbf{t}) = \alpha, \quad E_{\theta_0}(U\phi_4(U,\mathbf{T})|\mathbf{T}=\mathbf{t}) = \alpha E_{\theta_0}(U|\mathbf{T}=\mathbf{t})\ .$$

For a proof see Lehmann[2]

For an application, consider the test of independence in a 2×2 contingency table

X_{11}	X_{12}	X_{1+}
X_{21}	X_{22}	X_{2+}
X_{+1}	X_{+2}	N

[2]E.L.Lehmann (1991), *Testing Statistical Hypotheses, Second Edition* Wadsworth & Brooks/Cole, Pages 145-149.

where for integer x_{ij}

$$P(X_{11} = x_{11}, X_{12} = x_{12}, X_{21} = x_{21}) = \frac{N!}{x_{11}!x_{12}!x_{21}!x_{22}!} p_{11}^{x_{11}} p_{12}^{x_{12}} p_{21}^{x_{21}} p_{22}^{x_{22}} \tag{12.9}$$

and

$$\sum_{j=1}^{2} x_{ij} = x_{i+} \quad \sum_{i=1}^{2} x_{ij} = x_{+j} \quad \sum_{j=1}^{2} p_{ij} = p_{i+} \quad \sum_{i=1}^{2} p_{ij} = p_{+j} \text{ for } i, j = 1, 2,$$

$$x_{ij} \geq 0, \quad p_{ij} \geq 0, \quad \sum_{i=1}^{2}\sum_{j=1}^{2} x_{ij} = N, \text{ and } \sum_{i=1}^{2}\sum_{j=1}^{2} p_{ij} = 1.$$

The hypothesis is $H: \ p_{ij} = p_{i+}p_{+j}$ for all $i, j = 1, 2$ vs. $A: \ p_{ij} \neq p_{i+}p_{+j}$ for sone $i, j \in \{1, 2\}$. If we write

$$\theta = \ln\left(\frac{p_{21}p_{12}}{p_{11}p_{22}}\right)$$

then

$$p_{11} = p_{1+}p_{+1} + \frac{(1 - p_{21}p_{12}/(p_{11}p_{22}))}{p_{21}p_{12}/(p_{11}p_{22})} p_{21}p_{12} = p_{1+}p_{+1} + \frac{(1 - e^{\theta})}{e^{\theta}} p_{21}p_{12}$$

and

$$p_{ij} = p_{i+}p_{+j} + (-1)^{i+j}\frac{(1 - e^{\theta})}{e^{\theta}} p_{21}p_{12} \text{ for } i, j = 1, 2.$$

Then we can rewrite equation (12.9) as

$$\exp\{-x_{11}\theta + x_{+1}\ln(p_{12}/p_{22}) + x_{+1}\ln(p_{21}/p_{22}) + N\ln(p_{22})\}$$

and the hypothesis is equivalent to $H: \ \theta = 0$ vs. $A: \ \theta \neq 0$. The U.M.P. unbiased test then rejects with probability

$$\phi_4 = \begin{cases} 1 & \text{if } x_{11} < c_1(x_{1+}, x_{+1}) \text{ or } x_{11} > c_2(x_{1+}, x_{+1}) \\ \xi_i & \text{if } x_{11} = c_i(x_{1+}, x_{+1}) \text{ for } i = 1, 2 \\ 0 & \text{if } c_1(x_{1+}, x_{+1}) < x_{11} < c_2(x_{1+}, x_{+1}) \end{cases}$$

where the conditional probability under the hypothesis is

$$P_H(X_{11} = x_{11}|x_{1+}, x_{+1}) = \frac{\begin{pmatrix} x_{1+} \\ x_{11} \end{pmatrix}\begin{pmatrix} x_{2+} \\ x_{+1} - x_{11} \end{pmatrix}}{\begin{pmatrix} N \\ x_{+1} \end{pmatrix}}$$

and c_1, c_2, ξ_1, and ξ_2 satisfy

$$E_H(\phi_4|x_{1+}, x_{+1}) = \alpha \ , \quad E_H(X_{11}\phi_4|x_{1+}, x_{+1}) = \alpha E_H(X_{11}|x_{1+}, x_{+1}).$$

We solve the following 2 equations for c_1, c_2, ξ_1, and ξ_2 by trial and error

$$\sum_{x_{11}} \phi_4 \frac{\begin{pmatrix} x_{1+} \\ x_{11} \end{pmatrix} \begin{pmatrix} x_{2+} \\ x_{+1} - x_{11} \end{pmatrix}}{\begin{pmatrix} N \\ x_{+1} \end{pmatrix}} = \alpha$$

$$\sum_{x_{11}} \phi_4 \frac{\begin{pmatrix} x_{1+} - 1 \\ x_{11} - 1 \end{pmatrix} \begin{pmatrix} x_{2+} \\ x_{+1} - x_{11} \end{pmatrix}}{\begin{pmatrix} N - 1 \\ x_{+1} - 1 \end{pmatrix}} = \alpha \ .$$

If $F(x|N, D, n)$ is the hypergeometric c.d.f., $p(x|N, D, n)$ is the p.d.f. given in chapter 3, and $F((a, b]|N, D, n) = F(b|n, D, n) - F(a|N, D, n)$ is the interval probability, then we solve for c_1, c_2 by trial and error to satisfy

$$F((c_1, c_2 - 1]|N, x_{1+}, x_{+1}) \leq 1 - \alpha$$

$$F((c_1 - 1, c_2]|N, x_{1+}, x_{+1}) > 1 - \alpha$$

$$F((c_1 - 1, c_2 - 2]|N - 1, x_{1+} - 1, x_{+1} - 1) \leq 1 - \alpha$$

$$F((c_1 - 2, c_2 - 1]|N - 1, x_{1+} - 1, x_{+1} - 1) > 1 - \alpha$$

and then solve for ξ_1, ξ_2 from

$$(1 - \xi_1)p(c_1|N, x_{1+}, x_{+1}) + (1 - \xi_2)p(c_2|N, x_{1+}, x_{+1}) =$$

$$1 - \alpha - F((c_1, c_2 - 1]|N, x_{1+}, x_{+1}))$$

$$(1-\xi_1)p(c_1-1|N-1, x_{1+}-1, x_{+1}-1)+(1-\xi_2)p(c_2-1|N-1, x_{1+}-1, x_{+1}-1) =$$

$$1 - \alpha - F((c_1 - 1, c_2 - 2]|N - 1, x_{1+} - 1, x_{+1} - 1).$$

If the constraints that $0 \leq \xi_1, \xi_2 \leq 1$ are not satisfied, iteration continues on c_1, c_2 until they are.

For the case of a continuous distribution, if there exists a statistic V for the uniformly most powerful test of theorem (12.4) that is monotone in U

and statistically independent of $\mathbf{T}$ under the hypothesis H, then V can be used for an unconditional test.

Basu's[3] theorem can be used in many cases to show statistical independence.

Theorem 12.5 *Let T be sufficient for $\mathcal{P} = \{P_\theta : \theta \in \Theta\}$ with $\mathcal{P}^T$ boundedly complete. If V is any statistic that does not depend on θ then V is independent of T.*

Proof. By assumption $E_\theta \phi(V)$ is independent of θ for any critical function ϕ. By bounded completeness, all similar tests have Neyman structure using theorem 12.3. Thus $E(\phi(V)|T)$ is constant for every bounded function ϕ and we have independence.$\blacksquare$

As an illustration, consider the regression model $\mathbf{Y} = \mathbf{X}\beta + \varepsilon$ given in equation (11.3) and the problem of testing $H: \ \psi = \sum_{i=1}^p a_i\beta_i = \psi_0$ vs. $A: \psi \neq \psi_0$. Using the $\mathbf{X} = \mathbf{QR}$ decomposition where $\mathbf{Q}^{n\times n} = (\mathbf{Q}_1^{n\times p}, \mathbf{Q}_2^{n\times(n-p)})$ is orthogonal and

$$\mathbf{R}^{n\times p} = \begin{pmatrix} r_{11} & r_{12} & r_{13} & \dots & r_{1p} \\ 0 & r_{22} & r_{23} & \dots & r_{2p} \\ 0 & 0 & r_{33} & \dots & r_{3p} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & r_{pp} \\ 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{R}_{11}^{p\times p} \\ \mathbf{0} \end{pmatrix}$$

where $r_{ii} > 0$ we form the orthogonal matrix

$$\mathbf{D}^{p\times p} = \begin{pmatrix} \mathbf{d}_1^T \\ \mathbf{d}_2^T \\ \vdots \\ \mathbf{d}_p^T \end{pmatrix}$$

where

$$\mathbf{d}_1^T = \mathbf{a}^T\mathbf{R}_{11}^{-1}/(\mathbf{a}^T\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T}\mathbf{a})^{1/2}, \quad \mathbf{D}^T\mathbf{D} = \mathbf{I}_p = \mathbf{D}\mathbf{D}^T \ .$$

[3]Basu, D. (1955). On statistics independent of a complete sufficient statistic. *Sankhyā* **15**, 577-580.

Making the transformations

$$\mathbf{Z}^{p\times 1} = \mathbf{Q}_1^T\mathbf{Y}, \quad \mathbf{W}^{(n-p)\times 1} = \mathbf{Q}_2^T\mathbf{Y}$$

$$\mathbf{U} = \mathbf{D}\mathbf{Z} = \begin{pmatrix} U_1 \\ U_2 \\ \vdots \\ U_p \end{pmatrix} = \begin{pmatrix} \hat{\psi}/(\mathbf{a}^T\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T}\mathbf{a})^{1/2} \\ \mathbf{d}_2^T\mathbf{Z} \\ \vdots \\ \mathbf{d}_p^T\mathbf{Z} \end{pmatrix}$$

we have the joint density

$$f_{\mathbf{U},\mathbf{W}}(\mathbf{u},\mathbf{w}) = \frac{1}{(\sigma\sqrt{2\pi})^n}\exp\left\{-\frac{1}{2\sigma^2}[(\mathbf{u}-E(\mathbf{U}))^T(\mathbf{u}-E(\mathbf{U}))+\mathbf{w}^T\mathbf{w}]\right\}$$

$$= C\exp\left\{\frac{\psi\hat{\psi}}{\sigma^2(\mathbf{a}^T\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T}\mathbf{a})} + \sum_{i=2}^{p}\nu_i u_i - \frac{1}{2\sigma^2}(\mathbf{u}^T\mathbf{u}+\mathbf{w}^T\mathbf{w})\right\}$$

where $\nu_i = \mathbf{d}_i^T\mathbf{R}_{11}\beta/\sigma^2$ for $i = 2, 3, \ldots, p$ and $\mathbf{u}^T\mathbf{u}+\mathbf{w}^T\mathbf{w} = \mathbf{y}^T\mathbf{y}$.
Applying theorem (12.4) part (4) using $\theta = \psi/(\sigma^2\mathbf{a}^T\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T}\mathbf{a})$ the U.M.P. unbiased test is

$$\phi_4 = \begin{cases} 1 \text{ if } \hat{\psi} < c_1(\mathbf{t}) \text{ or } \hat{\psi} > c_2(\mathbf{t}) \\ \xi_{4i}(\mathbf{t}) \text{ if } \hat{\psi} = c_i(\mathbf{t}) \quad i = 1,2 \\ 0 \text{ if } c_1(\mathbf{t}) < \hat{\psi} < c_2(\mathbf{t}) \end{cases}$$

where $\mathbf{t} = ((u_2, u_3, \ldots, u_p), \mathbf{y}^T\mathbf{y})$ and

$$E_{\theta_0}(\phi_4|\mathbf{t}) = \alpha, \quad E_{\theta_0}(\hat{\psi}\phi_4|\mathbf{t}) = \alpha E_{\theta_0}(\hat{\psi}|\mathbf{t}) \ .$$

Equivalently, the U.M.P. unbiased test rejects if $V =$

$$\frac{[U_1 - \psi_0/(\mathbf{a}^T\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T}\mathbf{a})^{1/2}]}{\left(\frac{1}{(n-p)}\{\mathbf{Y}^T\mathbf{Y} - U_1^2 - \sum_{i=2}^{p}U_i^2\}\right)^{1/2}} = \frac{(\hat{\psi}-\psi_0)}{\hat{\sigma}(\mathbf{a}^T\mathbf{R}_{11}^{-1}\mathbf{R}_{11}^{-T}\mathbf{a})^{1/2}} \notin (-t_{n-p,\alpha/2}(0), t_{n-p,\alpha/2}(0))$$

since V is monotone in $\hat{\psi}$ and statistically independent of $\mathbf{t}$ under H. Here $t_{n-p,\alpha/2}(0))$ is the upper $\alpha/2$ percentage point of the central Student t distribution with degrees of freedom parameter $n-p$.

12.2.6 P-values for UMPU Tests

Definition 12.3 *The P-value, for a test based on the statistic T, is the smallest value of α for which the observed value of T always leads to the rejection of the null hypothesis.*

Equivalently, this extended P-value is the smallest value of the significance level α for which the observed value of T rejects with probability 1. For conditional tests, we use the conditional significance levels in the definition, given the value of the complete sufficient statistic under the null hypothesis.

Under our definition, in a two-sided setting, we do not allow randomization at the observed value of the test statistics but do allow possible randomization in the other tail for discrete distributions.

To illustrate, consider X binomial(n, p) and $H : p = p_0$ versus $A : p \neq p_0$. Then the equations determining ϕ_4 for the UMPU test reduce to

$$\sum_{x=0}^{C_1-1} f_{\mathcal{B}}(x|n, p_0) + \xi_1 f_{\mathcal{B}}(C_1|n, p_0) + \xi_2 f_{\mathcal{B}}(C_2|n, p_0) + \sum_{x=C_2+1}^{n} f_{\mathcal{B}}(x|n, p_0) = \alpha \tag{12.10}$$

$$\sum_{x=0}^{C_1-1} x f_{\mathcal{B}}(x|n, p_0) + \xi_1 C_1 f_{\mathcal{B}}(C_1|n, p_0) + \xi_2 C_2 f_{\mathcal{B}}(C_2|n, p_0) + \sum_{x=C_2+1}^{n} x f_{\mathcal{B}}(x|n, p_0) = \alpha n p_0 \tag{12.11}$$

where the binomial discrete density is

$$f_{\mathcal{B}}(x|n, p) = \binom{n}{x} p^x (1-p)^{n-x} \text{ for } x = 0, 1, \ldots, n,\ 0 < p < 1\ .$$

To solve these two equations for (C_1, C_2), (ξ_1, ξ_2) we first iterate on C_1, C_2 so that both

$$\sum_{x=C_1+1}^{C_2-1} f_{\mathcal{B}}(x|n, p_0) \leq 1 - \alpha, \quad \sum_{x=C_1}^{C_2} f_{\mathcal{B}}(x|n, p_0) > 1 - \alpha$$

and

$$\sum_{x=C_1+1}^{C_2-1} f_{\mathcal{B}}(x-1|n-1, p_0) \leq 1 - \alpha, \quad \sum_{x=C_1}^{C_2} f_{\mathcal{B}}(x|n, p_0) > 1 - \alpha$$

and then solve the two linear equations for $\xi_1, \xi_2)$ from

$$(1-\xi_1)f_{\mathcal{B}}(C_1|n,p_0)+(1-\xi_2)f_{\mathcal{B}}(C_2|n,p_0)=1-\alpha-\sum_{x=C_1+1}^{C_2-1} f_{\mathcal{B}}(x|n,p_0)$$

$$(1-\xi_1)f_{\mathcal{B}}(C_1-1|n-1,p_0)+(1-\xi_2)f_{\mathcal{B}}(C_2-1|n-1,p_0)=1-\alpha-\sum_{x=C_1}^{C_2-2} f_{\mathcal{B}}(x|n-1,p_0)\ . \tag{12.12}$$

If ξ_1 or $\xi_2 \notin [0,1]$ we iterate again on C_1, C_2 until $0 \le \xi_1, \xi_2 \le 1$. Some care must be taken in obtaining the numerical solutions to the two equations (12.12). We found multiple solutions but only one where $0 \le \xi_1, \xi_2 \le 1$.

For the P-value calculation, define m to be the mode of the binomial(n, p_0) distribution where $m = \lfloor (n+1)p_0 \rfloor$ is the greatest integer not exceeding $(n+1)p_0$. Then for observed value $X = x$ we calculate

$$\hat{\alpha}(x) = P_H(X < C_1) + \xi_1 P_H(X = C_1) + \xi_2 P_H(X = C_2) + P_H(X > C_2)$$

where $C_i = C_i(x)$, and $\xi_i = \xi_i(x)$, $i = 1, 2$, are determined as follows:
If $x < m$ set $C_1 = x$, $\xi_1 = 1$ and solve for C_2 and ξ_2 from

$$1-\xi_2 = \frac{\sum_{x=C_1}^{C_2-2} f_{\mathcal{B}}(x|n-1,p_0) - \sum_{x=C_1+1}^{C_2-1} f_{\mathcal{B}}(x|n,p_0)}{(f_{\mathcal{B}}(C_2|n,p_0) - f_{\mathcal{B}}(C_2-1|n-1,p_0))}$$

We start iterating with $C_2 = n$ and decerment it until $0 \le \xi_2 \le 1$.
If $x = m$ we set $\hat{\alpha}(m) = 1$.
If $x > m$ set $C_2 = 1$, $\xi_2 = 1$ and solve for C_1 and ξ_1 from

$$1-\xi_1 = \frac{\sum_{x=C_1}^{C_2-2} f_{\mathcal{B}}(x|n-1,p_0) - \sum_{x=C_1+1}^{C_2-1} f_{\mathcal{B}}(x|n,p_0)}{(f_{\mathcal{B}}(C_1|n,p_0) - f_{\mathcal{B}}(C_1-1|n-1,p_0))}\ .$$

We start with $C_1 = 0$ and increment it until $0 \le \xi_1 \le 1$.

For example, with $(x, n, p_0) = (3, 10, 0.6)$ we find $(C_1, C_2) = ((3, 8)$, $(\xi_1, \xi_2) = (1, 0.13745)$, and the P-value $\hat{\alpha}(3) = 0.11774$.

If X has a Poisson(λ) density

$$f_{\mathcal{P}}(x|\lambda) = \frac{\lambda^x e^{-\lambda}}{x!} \text{ for } x = 0, 1, 2, \ldots, \infty$$

for testing $H : \lambda = \lambda_0$ versus $A : \lambda \neq \lambda_0$ using the UMPU test, we proceed as in the binomial but with $f_{\mathcal{B}}(x|n, p_0)$ and $f_{\mathcal{B}}(x-1|n-1, p_0)$ replaced by

$f_{\mathcal{P}}(x|\lambda_0)$ and $f_{\mathcal{P}}(x-1|\lambda_0)$ and $m = \lfloor \lambda_0 \rfloor$.
For $x < m$ we can start iteration with $C_2 = 3m$ and decrement it until $0 \le \xi_2 \le 1$.

For example, if $(x, \lambda_0) = (13, 7.0)$ then $(C_1, C_2) = (3, 13)$, $(\xi_1, \xi_2) = (0.134575, 1)$, and the P-value $\hat{\alpha}(13) = 0.063651$.

If X has the negative binomial(r, p) distribution with density

$$f_{\mathcal{NB}}(x|r,p) = \begin{pmatrix} r+x-1 \\ x \end{pmatrix} p^r(1-p)^x \text{ for } x = 0, 1, 2, \ldots, \infty,\ 0 < p < 1,\ r \ge 1$$

for testing $Hp = p_0$ versus $A : p \ne p_0$ using the UMPU test we proceed similarly replacing $f_{\mathcal{B}}(x|n, p_0)$ and $f_{\mathcal{B}}(x-1|n-1, p_0)$ by $f_{\mathcal{NB}}(x|r, p_0)$ and $f_{\mathcal{NB}}(x-1|r+1, p_0)$ with mode $m = \lfloor (r-1)(1-p_0)/p_0 \rfloor$. We iterate as in the Poisson.

For example, for $(x, r, p_0) = (14, 10, 0.6)$ we get $(C_1, C_2) = (2, 14)$, $(\xi_1, \xi_2) = (0.53209, 1)$ and P-value $\hat{\alpha}(14) = 0.093468$.

If X has a binomial(n_1, p_1) distribution and Y has a binomial(n_2, p_2) distribution and X, Y are independent, then the P-value for the UMPU test (conditional on $X + Y = s$) of $H : p_1 = p_2$ versus $A : p_1 \ne p_2$ is obtained from the hypergeometric conditional distribution

$$f_{\mathcal{H}}(x|N, s, n_1) = \begin{pmatrix} n_1 \\ x \end{pmatrix} \frac{(s)_x (N-s)_{(n_1-x)}}{(N)_{n_1}} \text{ for } x = L, L+1, \ldots, U$$

where $N = n_1 + n_2$, $(a)_k = \prod_{i=0}^{k-1}(a-i)$, $L = \max(0, s-n_2)$, and $U = \min(n_1, s)$. We replace $f_{\mathcal{B}}(x|n, p_0)$ and $f_{\mathcal{B}}(x-1|n-1, p_0)$ by $f_{\mathcal{H}}(x|N, s, n_1)$ and $f_{\mathcal{H}}(x-1|N-1, s-1, n_1-1)$ with mode $m = \lfloor (n_1+1)(s+1)/(N+2) \rfloor$. For $x < m$, we start iteration with $C_2 = U$ and decrement it until $0 \le \xi_2 \le 1$. For $x > m$, we start iteration with $C_1 = L$ and increment it until $0 \le \xi_1 \le 1$.

For example, if $(x, n_1) = (5, 15)$ and $(y, n_2) = (8, 9)$ then $(C_1, C_2) = (5, 11)$, $(\xi_1, \xi_2) = (1, 0.51793)$ and the P-value is $\hat{\alpha}(5) = 0.02333$.

The C++ program **Pvalue.cpp** in **Appendix E** calculates P-values for some discrete UMPU tests.

For a one sided test or a test that rejects for a statistic $T(X) \ge C$ the P-value $\hat{\alpha}(t) = P_H(T(X) \ge t)$ where t is the observed value of $T(X)$.

For continuous distributions, the P-value can usually be reduced to that of rejection for a statistic $T(X) \ge C$.
For example, let $X_1, X_2, \ldots, X_m$ $\mathcal{N}(\mu, \sigma^2)$ and $Y_1, Y_2, \ldots, Y_n$ $\mathcal{N}(\eta, \tau^2)$ all be

independent. For testing $H : \sigma^2 = \tau^2$ versus $A : \sigma^2 \neq \tau^2$ the UMPU test rejects for

$$V = \frac{\sum_{i=1}^m (X_i - \bar{X})^2}{\sum_{i=1}^m (X_i - \bar{X})^2 + \sum_{j=1}^n (Y_j - \bar{Y})^2} \notin [C_1, C_2]$$

where

$$\frac{\Gamma((m+n-2)/2)}{\Gamma((m-1)/2)\Gamma((n-1)/2)} \int_{C_1}^{C_2} v^{(m-1)/2-1}(1-v)^{(n-1)/2-1} dv = 1 - \alpha$$

and

$$C_1^{m-1}(1-C_1)^{n-1} = C_2^{m-1}(1-C_2)^{n-1}$$

Then for v the observed value of V we have the P-value

$$\hat{\alpha}(v) = P_H(V^{m-1}(1-V)^{n-1} \leq v^{m-1}(1-v)^{n-1}) \ .$$

12.3 Generalized Likelihood Ratio Test $-2\log(\Lambda)$.

In situations with composite hypotheses where no UMP or UMPU test exists, the generalized likelihood ratio test of Wilks(1938)[4] is often used. If the parameter space is Θ and the hypothesis space is Θ_0 then the statistic is

$$-2\log_e(\Lambda) = 2[\ln(\sup_{\theta\in\Theta} f_X(x|\theta)) - \ln(\sup_{\theta\in\Theta_0} f_X(x|\theta))]$$

where $f_X(x|\theta)$ is the joint density of the observations with respect to a measure.

For example, consider the $r \times c$ contingency table

$$\mathbf{X} = \begin{pmatrix} X_{11} & X_{12} & \dots & X_{1c} \\ X_{21} & X_{22} & \dots & X_{2c} \\ \vdots & \vdots & \ddots & \vdots \\ X_{r1} & X_{r2} & \dots & X_{rc} \end{pmatrix}$$

with joint density

$$f_{\mathbf{X}}(\mathbf{x}|\mathbf{p}) = \frac{N!}{x_{11}!x_{12}!\cdots x_{rc}!} p_{11}^{x_{11}} p_{12}^{x_{12}} \cdots p_{rc}^{x_{rc}}$$

[4]Wilks, S.S.(1938) The large sample distribution of the likelihood ratio for testing composite hypotheses. *Annals of Mathematical Statistics* **9**, 60-62.

where $p_{ij} \in [0,1]$ and $\sum_{i=1}^{r}\sum_{j=1}^{c} p_{ij} = 1$. For testing the hypothesis $H : p_{ij} = p_{i+}p_{+j}$ for all i,j versus $A : p_{ij} \neq p_{i+}p_{+j}$ for some i,j where $p_{i+} = \sum_{j=1}^{c} p_{ij}$ and $p_{+j} = \sum_{i=1}^{r} p_{ij}$, the generalized likelihood ratio statistic is

$$-2\ln(\Lambda) = 2[\sum_{i=1}^{r}\sum_{j=1}^{c} X_{ij}\ln(X_{ij}/N) - \sum_{i=1}^{r} X_{i+}\ln(X_{i+}/N) - \sum_{j=1}^{c} X_{+j}\ln(X_{+j}/N)] \ .$$

The limiting distribution of $-2\ln(\lambda)$ under suitable regularity conditions is that of a chi square random variable. Davidson and Lever (1970) [5] give conditions and a proof of the asymptotic chi square distribution.

Let $\mathbf{X_i}$, $i = 1, 2, \ldots, n$ be independent, identically distributed with density $f(\mathbf{x_i}|\theta)$ with respect to a measure μ.

$$\mathbf{X_i} = \begin{pmatrix} X_{i1} \\ X_{i2} \\ \vdots \\ X_{ip} \end{pmatrix}, \qquad \theta = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_s \end{pmatrix} \in \Theta$$

where Θ is an s-dimensional parameter space.
Assumptions.

A1 $\frac{\partial \ln(f)}{\partial \theta_j}$, $\frac{\partial^2 \ln(f)}{\partial \theta_j \partial \theta_k}$, and $\frac{\partial^3 \ln(f)}{\partial \theta_j \partial \theta_k \partial \theta_t}$ exist for almost all $\mathbf{x} \in R^p$ and all $\theta \in \Theta$.

A2 For almost all $\mathbf{x}$ and all $\theta \in \Theta$

$$\left|\frac{\partial f}{\partial \theta_j}\right| < F_j(\mathbf{x}), \qquad \left|\frac{\partial^2 f}{\partial \theta_j \partial \theta_k}\right| < F_{jk}(\mathbf{x})$$

where $F_j(\mathbf{x})$ and $F_{jk}(\mathbf{x})$ are integrable over R^p for $j, k = 1, 2, \ldots, s$.

A3 For every $\theta \in \Theta$, the information matrix

$$\mathcal{I}(\theta) = E_\theta\left(\frac{\partial \ln(f(\mathbf{X}|\theta))}{\partial \theta}\frac{\partial \ln(f(\mathbf{X}|\theta))}{\partial \theta^T}\right)$$

is positive definite with finite determinant.

[5] Davidson and Lever (1970). The limiting distribution of the likelihood ratio statistic under a class of local alternatives. *Sankhya Ser. A* **32**, 209-224.

A4 For almost all $\mathbf{x} \in R^p$ and all $\theta \in \Theta$

$$\left| \frac{\partial^3 \ln(f(\mathbf{x}|\theta))}{\partial\theta_j \partial\theta_k \partial\theta_t} \right| < H_{jkt}(\mathbf{x})$$

where $E(H_{jkt}(\mathbf{X})) < M < \infty$ for some $M > 0$, $j, k, t = 1, 2, \ldots, s$.

B There exist positive numbers ν and T such that whenever

$$||\theta'' - \theta'|| = \sum_{j=1}^{s} |\theta''_j - \theta'_j| < \nu$$

for θ', $\theta'' \in \Theta$ we have

$$E_{\theta'} \left(\frac{\partial^2 \ln(f(\mathbf{X}|\theta''))}{\partial\theta''_j \partial\theta''_k} \right)^2 < T$$

for $j, k = 1, 2, \ldots, s$.

C There exist positive numbers η, K such that

$$E_\theta \left| \frac{\partial \ln(f(\mathbf{X}|\theta))}{\partial\theta_j} \right|^\eta < K$$

for all $\theta \in \Theta$, $j = 1, 2, \ldots, s$.

D There exist $\delta > 0$ and $L > 0$ such that

$$E_\theta(|H_{jkt}(\mathbf{X}) - E_\theta(H_{jkt}(\mathbf{X}))|^{1+\delta}) < L < \infty$$

for all $\theta \in \Theta$.

We consider a test of the composite hypothesis

$$H: \ \theta = \begin{pmatrix} \xi \\ \eta \end{pmatrix} = \begin{pmatrix} \xi_0 \\ \eta \end{pmatrix} = \theta^*$$

where

$$\xi_0 = \begin{pmatrix} \xi_{01} \\ \xi_{02} \\ \vdots \\ \xi_{0r} \end{pmatrix}, \quad \eta = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_{s-r} \end{pmatrix}$$

with ξ_0 completely specified, against *near-by* alternatives

$$A^{(n)}: \ \theta = \theta^{(n)} = \begin{pmatrix} \xi^{(n)} \\ \eta \end{pmatrix}$$

where $\xi^{(n)} = \xi_0 + \delta^{(n)}/\sqrt{n}$ and

$$\delta^{(n)} = \begin{pmatrix} \delta_1^{(n)} \\ \delta_2^{(n)} \\ \vdots \\ \delta_r^{(n)} \end{pmatrix} \to \begin{pmatrix} \delta_1 \\ \delta_2 \\ \vdots \\ \delta_r \end{pmatrix} \text{ as } n \to \infty.$$

Define

$$\mathcal{I}(\theta) = \begin{pmatrix} C_{11}^{r\times r}(\theta) & C_{12}(\theta) \\ C_{21}(\theta) & C_{22}^{(s-r)\times(s-r)} \end{pmatrix} = (c_{jk}(\theta) : j,k = 1,2,\ldots s)$$

$$\mathcal{I}^{-1}(\theta) = \begin{pmatrix} C^{11}(\theta) & C^{12}(\theta) \\ C^{21}(\theta) & C^{22}(\theta) \end{pmatrix}, \quad \bar{C}_{11}^{r\times r}(\theta) = (C^{11}(\theta))^{-1} .$$

Under the assumptions A,B,C,D we have the following

Theorem 12.6 *For testing the hypothesis $H : \theta = \theta^*$ versus $A^{(n)}$ the generalized likelihood ratio statistic*

$$-2\ln(\Lambda) \xrightarrow{\mathcal{L}} \chi_r^2(\lambda^2) \ \textit{as } n \to \infty$$

for a sequence of near-by alternatives $\theta = \theta^{(n)}$ where the limiting non centrality patameter $\lambda^2 = \delta^T \bar{C}_{11}(\theta^*)\delta$.

Sketch of proof.
Write the log likelihood

$$\mathcal{L}(\theta|X_1, X_2, \ldots, X_n) = \sum_{i=1}^{n} \ln(f(X_i|\theta))$$

and its derivatives

$$\left(\frac{\partial \mathcal{L}(\theta|X_1, X_2, \ldots, X_n)}{\partial \theta}\right)^{s\times 1} = \dot{\mathcal{L}}(\theta|X_1, X_2, \ldots, X_n)$$

$$\left(\frac{\partial^2 \mathcal{L}(\theta|X_1, X_2, \ldots, X_n)}{\partial\theta\partial\theta^T}\right)^{s\times s} = \ddot{\mathcal{L}}(\theta|X_1, X_2, \ldots, X_n)$$

Forming a limited Taylor expansion up to second order for $\theta^* \in \omega$ (the hypothesis space), and expanding about the maximum likelihood estimate under the general model gives

$$\mathcal{L}(\theta^*|X_1, X_2, \ldots, X_n) = \mathcal{L}(\hat{\theta}|X_1, X_2, \ldots, X_n) + (\hat{\theta} - \theta^*)^T \dot{\mathcal{L}}(\hat{\theta}|X_1, X_2, \ldots, X_n)$$
$$+\frac{1}{2}((\hat{\theta} - \theta^*)^T \ddot{\mathcal{L}}(\bar{\theta}|X_1, X_2, \ldots, X_n)(\hat{\theta} - \theta^*) \tag{12.13}$$

where $\bar{\theta}$ lies on a line between θ^* and $\hat{\theta}$.

Because of the continuity of the likelihood (differentiable), we have the maximum likelihood estimate is a root of the likelihood equation and $\dot{\mathcal{L}}(\hat{\theta}|X_1, X_2, \ldots, X_n) = \mathbf{0}$ so that equation (12.13) reduces to

$$\mathcal{L}(\theta^*|X_1, X_2, \ldots, X_n) = \mathcal{L}(\hat{\theta}|X_1, X_2, \ldots, X_n)$$
$$+\frac{1}{2}(\hat{\theta} - \theta^*)^T \ddot{\mathcal{L}}(\bar{\theta}|X_1, X_2, \ldots, X_n)(\hat{\theta} - \theta^*) \tag{12.14}$$

Next expand $\mathcal{L}(\theta^*|X_1, X_2, \ldots, X_n)$ about $\hat{\theta}_\omega$, the MLE under the hypothesis,

$$\hat{\theta}_\omega = \begin{pmatrix} \xi_0 \\ \hat{\eta}_\omega \end{pmatrix}$$

and we similarly get

$$\mathcal{L}(\theta^*|X_1, X_2, \ldots, X_n) = \mathcal{L}(\hat{\theta}_\omega|X_1, X_2, \ldots, X_n)$$
$$+\frac{1}{2}(\hat{\eta}_\omega - \eta)^T \left(\ddot{\mathcal{L}}(\overline{\overline{\theta}}|X_1, X_2, \ldots, X_n)\right)_{22} (\hat{\eta}_\omega - \eta) \tag{12.15}$$

where

$$\left(\ddot{\mathcal{L}}(\overline{\overline{\theta}}|X_1, X_2, \ldots, X_n)\right)_{22} = \left(\frac{\partial^2 \mathcal{L}(\theta|X_1, X_2, \ldots, X_n)}{\partial\theta_j\partial\theta_k} \;:\; j, k = 1, 2, \ldots, s - r\right)\Bigg|_{\theta=\overline{\overline{\theta}}}$$

and $\overline{\overline{\theta}}$ lies between θ^* and $\hat{\theta}_\omega$.

Subtracting equation (12.15) from equation (12.14), multiplying by 2 and transposing quadratic terms we get

$$-2\ln(\Lambda) = 2\mathcal{L}(\hat{\theta}|X_1, X_2, \ldots, X_n) - 2\mathcal{L}(\hat{\theta}_H|X_1, X_2, \ldots, X_n) =$$

$$\sqrt{n}(\hat{\theta}-\theta^*)^T\left(-\frac{1}{n}\ddot{\mathcal{L}}(\bar{\theta}|X_1,X_2,\ldots,X_n)\right)\sqrt{n}(\hat{\theta}-\theta^*)$$

$$-\sqrt{n}(\hat{\eta}_H-\eta)^T\left(-\frac{1}{n}\ddot{\mathcal{L}}(\bar{\bar{\theta}}|X_1,X_2,\ldots,X_n)\right)_{22}\sqrt{n}(\hat{\eta}_H-\eta) \tag{12.16}$$

If $\theta=\theta^{(n)}$ is the true value of the parameter vector for the *near-by* alternatives, we have $\theta^{(n)}\to\theta^*$ and using consistency of the maximum likelihood estimators, we have $\hat{\theta}\to\theta^*$ and $\hat{\theta}_H\to\theta^*$ in probability as $n\to\infty$. By the uniform strong law of large numbers,

$$-\frac{1}{n}\ddot{\mathcal{L}}(\bar{\theta}|X_1,X_2,\ldots,X_n)\xrightarrow{P}\mathcal{I}(\theta^*)=\begin{pmatrix} C_{11}(\theta^*) & C_{12}(\theta^*)\\ C_{21}(\theta^*) & C_{22}(\theta^*)\end{pmatrix}$$

$$=(c_{jk}(\theta^*):j,k=1,2,\ldots,s)$$

and

$$\left(-\frac{1}{n}\ddot{\mathcal{L}}(\bar{\bar{\theta}}|X_1,X_2,\ldots,X_n)\right)_{22}\xrightarrow{P}C_{22}(\theta^*)\ .$$

Then $-2\ln(\Lambda)$ will have the limiting distribution of

$$\sum_{j=1}^{s}\sum_{k=1}^{s}Z_jZ_kc_{jk}(\theta^*)-\sum_{j=r+1}^{s}\sum_{k=r+1}^{s}Z_{\omega j}Z_{\omega k}c_{jk}(\theta^*) \tag{12.17}$$

where

$$\sqrt{n}(\hat{\theta}_j-\theta_j^*)\xrightarrow{D}Z_j \text{ for } j=1,2,\ldots,s$$

and

$$\sqrt{n}(\hat{\eta}_{\omega j}-\eta_j)\xrightarrow{D}Z_{\omega j+r} \text{ for } j=1,2,\ldots,s-r\ .$$

We next show that equation (12.17) is equivalent to

$$\sum_{j=1}^{r}\sum_{k=1}^{r}Z_jZ_k\bar{c}_{jk}(\theta^*)=\mathbf{Z}_{11}^T\bar{C}_{11}(\theta^*)\mathbf{Z}_{11}$$

where

$$\mathbf{Z}_{11}=\begin{pmatrix} Z_1\\ Z_2\\ \vdots\\ Z_r\end{pmatrix}:\mathcal{N}_r(\delta,C^{11}(\theta^*))$$

We do this using two more limited expansions about $\hat{\theta}$ and $\hat{\theta}_\omega$ with $\bar{\theta}$ between θ and $\hat{\theta}$, $\bar{\theta}_\omega$ between θ and $\hat{\theta}_\omega$,

$$-\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\frac{\partial \ln(f(X_i|\theta^*))}{\partial\theta_j} = 0 + \sum_{k=1}^{s}\sqrt{n}(\hat{\theta}_k - \theta_k^*)\left(-\frac{1}{n}\sum_{i=1}^{n}\frac{\partial^2 \ln(f(X_i|\bar{\theta}))}{\partial\theta_j\partial\theta_k}\right)$$

and

$$-\frac{1}{\sqrt{n}}\sum_{i=1}^{n}\frac{\partial \ln(f(X_i|\theta^*))}{\partial\theta_j} = 0 + \sum_{k=r+1}^{s}\sqrt{n}(\hat{\theta}_{\omega k} - \theta_k^*)\left(-\frac{1}{n}\sum_{i=1}^{n}\frac{\partial^2 \ln(f(X_i|\bar{\theta}_\omega))}{\partial\theta_j\partial\theta_k}\right) .$$

As $n \to \infty$ these equations become

$$Y_j = \sum_{k=1}^{s} Z_k c_{jk}(\theta^*) \text{ for } j = 1, 2, \ldots, s$$

and

$$Y_j = \sum_{k=r+1}^{s} Z_{\omega k} c_{jk}(\theta^*) \text{ for } j = r+1, r+2, \ldots, s$$

where

$$\mathbf{Y} = \begin{pmatrix} Y_1 \\ Y_2 \\ \vdots \\ Y_n \end{pmatrix} : \mathcal{N}_s(\mathbf{0}, \mathcal{I}(\theta^*))$$

using the central limit theorem.

Equation (12.17) can then be written

$$\mathbf{Z}^T\mathcal{I}(\theta^*)\mathbf{Z} - \mathbf{Z}_{\omega 22}^T C_{22}\mathbf{Z}_{\omega 22} \tag{12.18}$$

where

$$\mathbf{Z}^T = \mathbf{Y}^T\mathcal{I}^{-1}(\theta^*)$$

and for $\mathbf{Y}_{22}^T = (Y_{r+1}, Y_{r+2}, \ldots, Y_s) = \mathbf{Y}^T(\mathbf{0}, I_{s-r})$,

$$\mathbf{Z}_{\omega 22}^T = (Z_{\omega r+1}, Z_{\omega r+2}, \ldots, Z_{\omega s}) = \mathbf{Y}_{22}^T C_{22}^{-1} .$$

Substituting into equation (12.18) gives

$$\mathbf{Y}^T\left(\mathcal{I}^{-1} - \begin{pmatrix} 0 & 0 \\ 0 & C_{22}^{-1} \end{pmatrix}\right)\mathbf{Y} = \mathbf{Z}^T\mathcal{I}\left(\mathcal{I}^{-1} - \begin{pmatrix} 0 & 0 \\ 0 & C_{22}^{-1} \end{pmatrix}\right)\mathcal{I}\mathbf{Z}$$

$$= \mathbf{Z}^T \begin{pmatrix} C_{11} - C_{12}C_{22}^{-1}C_{21} & 0 \\ 0 & 0 \end{pmatrix} \mathbf{Z} = \mathbf{Z}_{11}^T (C^{11})^{-1} \mathbf{Z}_{11} \ .$$

Now $\mathbf{Z}_{11}^{r\times 1} = (Z_1, Z_2, \ldots, Z_r)^T : \mathcal{N}_r(\delta, C^{11})$ for the sequence of *near-by* alternatives so that

$$\mathbf{Z}_{11}^T (C^{11})^{-1} \mathbf{Z}_{11} : \chi_r^2(\lambda^2)$$

where the limiting noncentrality parameter

$$\lambda^2 = \delta^T (C^{11})^{-1} \delta = \delta^T \bar{C}_{11} \delta \ . \blacksquare$$

For an example, let $\mathbf{X}_i$ for $i = 1, 2, \ldots, n$ be independent bivariate normal

$$\mathbf{X}_i = \begin{pmatrix} X_{i1} \\ X_{i2} \end{pmatrix} : \mathcal{N}_2 \left(\begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix} \right) \ .$$

Consider the hypothesis

$$H : \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} = \begin{pmatrix} \mu_{01} \\ \mu_{02} \end{pmatrix} \text{ versus } A : \begin{pmatrix} \mu_1 \\ \mu_2 \end{pmatrix} \neq \begin{pmatrix} \mu_{01} \\ \mu_{02} \end{pmatrix} \ .$$

The maximum likelihood estimators under the general model are

$$\hat{\mu}_j = \bar{X}_j = \frac{\sum_{i=1}^n X_{i1j}}{n}, \quad \hat{\sigma}_j^2 = \frac{\sum_{i=1}^n (X_{ij} - \bar{X}_j)^2}{n} \text{ for } j = 1, 2$$

and

$$\hat{\rho} = \frac{\sum_{i=1}^n (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2)}{\left(\sum_{i=1}^n (X_{i1} - \bar{X}_1)^2 \sum_{i=1}^n (X_{i2} - \bar{X}_2)^2\right)^{1/2}}$$

The maximum likelihood estimators under the hypothesis are

$$\hat{\sigma}_{\omega j}^2 = \frac{\sum_{i=1}^n (X_{ij} - \mu_{0j})^2}{n} \text{ for } j = 1, 2$$

and

$$\hat{\rho}_\omega = \frac{\sum_{i=1}^n (X_{i1} - \mu_{01})(X_{i2} - \mu_{02})}{\left(\sum_{i=1}^n (X_{i1} - \mu_{01})^2 \sum_{i=1}^n (X_{i2} - \mu_{02})^2\right)^{1/2}}$$

The generalized likelihood ratio statistic

$$-2\ln(\Lambda) = n \ln \left(\frac{\hat{\sigma}_{\omega 1}^2 \hat{\sigma}_{\omega 2}^2 (1 - \hat{\rho}_\omega^2)}{\hat{\sigma}_1^2 \hat{\sigma}_2^2 (1 - \hat{\rho}^2)} \right) \ .$$

For $\theta = (\mu_1, \mu_2, \sigma_1, \sigma_2, \rho)^T$, the Fisher information matriz is

$$\mathcal{I}(\theta) = \begin{pmatrix} C_{11} & \mathbf{0} \\ \mathbf{0} & C_{22} \end{pmatrix}$$

where

$$C_{11} = \begin{pmatrix} 1/(\sigma_1^2(1-\rho^2)) & -\rho/(\sigma_1\sigma^2(1-\rho^2)) \\ -\rho/(\sigma_1\sigma_2(1-\rho^2)) & 1/(\sigma_2^2(1-\rho^2)) \end{pmatrix}$$

and

$$C_{22} = \begin{pmatrix} (2-\rho^2)/(4\sigma_1^4(1-\rho^2)) & -\rho^2/(4\sigma_1^2\sigma_2^2(1-\rho^2)) & -\rho/(\sigma_1^2(1-\rho^2)) \\ -\rho^2/(4\sigma_1^2\sigma_2^2(1-\rho^2)) & (2-\rho^2)/(4\sigma_2^4(1-\rho^2)) & -\rho/(\sigma_2^2(1-\rho^2)) \\ -\rho/(\sigma_1^2(1-\rho^2)) & -\rho/(\sigma_2^2(1-\rho^2)) & (1+\rho^2)/(1-\rho^2)^2 \end{pmatrix}.$$

The inverse is

$$\mathcal{I}^{-1}(\theta) = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 & 0 & 0 & 0 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 & 0 & 0 & 0 \\ 0 & 0 & 2\sigma_1^4 & 2\rho^2\sigma_1^2\sigma_2^2 & \rho(1-\rho^2)\sigma_1^2 \\ 0 & 0 & 2\rho^2\sigma_1^2\sigma_2^2 & 2\sigma_2^4 & \rho(1-\rho^2)\sigma_2^2 \\ 0 & 0 & \rho(1-\rho^2)\sigma_1^2 & \rho(1-\rho^2)\sigma_2^2 & (1-\rho^2)^2 \end{pmatrix}.$$

Thus because $C_{12} = \mathbf{0} = C_{21}$ we have

$$\bar{C}_{11} = C_{11} = \begin{pmatrix} 1/(\sigma_1^2(1-\rho^2)) & -\rho/(\sigma_1\sigma_2(1-\rho^2)) \\ -\rho/(\sigma_1\sigma_2(1-\rho^2)) & 1/(\sigma_2^2(1-\rho^2)) \end{pmatrix}$$

and

$$-2\ln(\Lambda) \xrightarrow{L} \chi_2^2(\lambda^2)$$

as $n \to \infty$ where the noncentrality parameter

$$\lambda^2 = \left[\frac{\delta_1^2}{\sigma_1^2(1-\rho^2)} - \frac{2\delta_1\delta_2\rho}{\sigma_1\sigma_2(1-\rho^2)} + \frac{\delta_2^2}{\sigma_2^2(1-\rho^2)}\right]$$

for the *near-by* alternatives $\mu_1 = \mu_{01} + \delta_1/\sqrt{n}$ and $\mu_2 = \mu_{02} + \delta_2/\sqrt{n}$.
We can write (see for example Anderson (1958)[6])

$$-2\ln(\Lambda) = n\ln(1 + T^2/(n-1))$$

[6] Anderson, T.W. (1958) *An Introduction to Multivariate Statistical Analysis.* J. Wiley and Sons, Inc. New York pages 102-103.

where Hotelling's

$$T^2 = n^2(n-1)(\bar{X}_1 - \mu_{01}, \bar{X}_2 - \mu_{02}) \begin{pmatrix} \hat{\sigma}_1^2 & \hat{\rho}\hat{\sigma}_1\hat{\sigma}_2 \\ \hat{\rho}\hat{\sigma}_1\hat{\sigma}_2 & \hat{\sigma}_2^2 \end{pmatrix}^{-1} \begin{pmatrix} \bar{X}_1 - \mu_{01} \\ \bar{X}_2 - \mu_{02} \end{pmatrix}$$

$$= n((\bar{\mathbf{X}} - \mu_0)^T \mathbf{S}^{-1} (\bar{\mathbf{X}} - \mu_0) \ .$$

Here

$$\mathbf{S} = \frac{1}{n-1} \begin{pmatrix} \sum_{i=1}^n (X_{i1} - \bar{X}_1)^2 & \sum_{i=1}^n (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2) \\ \sum_{i=1}^n (X_{i1} - \bar{X}_1)(X_{i2} - \bar{X}_2) & \sum_{i=1}^n (X_{i2} - \bar{X}_2)^2 \end{pmatrix}$$

and $T^2(n-1)/(2n)$ has the noncentral $F_{2,n-1}(\lambda^2)$ distribution with noncentrality parameter

$$\lambda^2 = n(\mu_1 - \mu_{01}, \mu_2 - \mu_{02}) \frac{1}{(1-\rho^2)} \begin{pmatrix} 1/\sigma_1^2 & -\rho/(\sigma_1\sigma_2) \\ -\rho/(\sigma_1\sigma_2) & 1/\sigma_2^2 \end{pmatrix} \begin{pmatrix} \mu_1 - \mu_{01} \\ \mu_2 - \mu_{02} \end{pmatrix}$$

$$= n \left[\frac{(\mu_1 - \mu_{01})^2}{\sigma_1^2(1-\rho^2)} - \frac{2(\mu_1 - \mu_{01})(\mu_2 - \mu_{02})\rho}{\sigma_1\sigma_2(1-\rho^2)} + \frac{(\mu_2 - \mu_{02})^2}{\sigma_2^2(1-\rho^2)} \right]$$

which is the same as λ^2 given above with $\delta_j = \sqrt{n}(\mu_j - \mu_{0j})$, $j = 1, 2$.
We note that the exact distribution converges to the asymptotic distribution

$$n \ln\left(1 + \frac{T^2}{n-1}\right) = \frac{n}{n-1} T^2 + O_p(\frac{1}{n})$$

$$= \frac{n}{n-1} \left[F_{2,n-1}(\lambda^2) \frac{2n}{n-1} \right] + O_p(\frac{1}{n}) \xrightarrow{L} \chi_2^2(\lambda^2)$$

as $n \to \infty$.

Often the hypothesis is not stated in the form $H : \theta = (\xi_0, \eta)^T$ but can be brought into this form by a transformation that gives

$$H : \zeta(\theta) = \zeta^* = \begin{pmatrix} \xi_0 \\ \eta \end{pmatrix} \ .$$

Davidson and Lever[4] give the following conditions for

$$-2\ln(\Lambda) \xrightarrow{L} \chi_r^2(\lambda^2)$$

for *near-by* alternatives $\xi = \xi_0 + \delta^{(n)}/\sqrt{n}$, $\delta^{(n)} \to \delta = (\delta_1, \delta_2, \ldots, \delta_r)^T$.
Assumptions

(a) The inverse

$$\theta(\zeta) = \begin{pmatrix} \theta_1(\zeta) \\ \theta_2(\zeta) \\ \vdots \\ \theta_r(\zeta) \\ \eta_1(\zeta) \\ \vdots \\ \eta_{s-r}(\zeta) \end{pmatrix} \text{ exists where } \zeta = \zeta(\theta) = \begin{pmatrix} \xi_1(\theta) \\ \xi_2(\theta) \\ \vdots \\ \xi_r(\theta) \\ \eta_1(\theta) \\ \vdots \\ \eta_{s-r}(\theta) \end{pmatrix} .$$

(b) The first and second partial derivatives $\partial\theta(\zeta)/(\partial\zeta_j)$, $\partial^2\theta(\zeta)/(\partial\zeta_j\partial\zeta_k)$ exist and are bounded.

(c) $\inf_{\theta\in\Theta} \left|\partial\zeta/(\partial\theta^T)\right| > 0$.

The noncentrality parameter

$$\lambda^2 = \delta^T \bar{C}_{11}(\zeta^*)\delta$$

where

$$\mathcal{I}(\zeta^*) = \left(-E\left(\frac{\partial^2 \ln(f)}{\partial\zeta_j\partial\zeta_k}\right)\Bigg|_{\zeta=\zeta^*} : j,k = 1,2,\ldots,s \right) = \begin{pmatrix} C_{11}^{r\times r}(\zeta^*) & C_{12}(\zeta^*) \\ C_{21}(\zeta^*) & C_{22}^{(s-r)\times(s-r)}(\zeta^*) \end{pmatrix}$$

$$\mathcal{I}^{-1}(\zeta^*) = \begin{pmatrix} C^{11}(\zeta^*) & C^{12}(\zeta^*) \\ C^{21}(\zeta^*) & C^{22}(\zeta^*) \end{pmatrix} \text{ and } \bar{C}_{11}(\zeta^*) = (C^{11}(\zeta^*))^{-1} .$$

If we have already calculated the information matrix $\mathcal{I}(\theta)$ then we can calculate

$$\mathcal{I}(\zeta) = \left(\frac{\partial\theta^T}{\partial\zeta}\right)\mathcal{I}(\theta)\left(\frac{\partial\theta}{\partial\zeta^T}\right)$$

where

$$\frac{\partial\theta}{\partial\zeta^T} = \begin{pmatrix} \frac{\partial\theta_1}{\partial\zeta_1} & \cdots & \frac{\partial\theta_1}{\partial\zeta_s} \\ \vdots & \ddots & \vdots \\ \frac{\partial\theta_s}{\partial\zeta_1} & \cdots & \frac{\partial\theta_s}{\partial\zeta_s} \end{pmatrix} \text{ and } \frac{\partial\theta^T}{\partial\zeta} = \left(\frac{\partial\theta}{\partial\zeta^T}\right)^T .$$

Consider the example of testing the hypothesis $H : \mu_1 = \mu_2$ and $\sigma_1^2 = \sigma_2^2$ versus the alternative $A : \mu_1 \neq \mu_2$ or $\sigma_1^2 \neq \sigma_2^2$ with independent

$$\begin{pmatrix} X_{i1} \\ X_{i2} \end{pmatrix} : \mathcal{N}_2\left(\begin{pmatrix} \mu_1 \\ \mu_1 \end{pmatrix}, \begin{pmatrix} \sigma_1^2 & 0 \\ 0 & \sigma_2^2 \end{pmatrix}\right) \text{ for } i = 1,2,\ldots,n .$$

The maximum liklihood estimators under the general model are

$$\hat{\mu_j} = \frac{1}{n}\sum_{i=1}^{n} X_{ij} = \bar{X}_j, \quad \hat{\sigma}_j^2 = \frac{1}{n}\sum_{i=1}^{n}(X_{ij} - \bar{X}_j)^2 \text{ for } j = 1, 2\,.$$

Under the hypothesis,

$$\hat{\mu}_\omega = (\bar{X}_1 + \bar{X}_2)/2, \quad \hat{\sigma}_\omega^2 = \frac{1}{2n}\left(\sum_{i=1}^{n}[(X_{i1} - \hat{\mu}_\omega)^2 + (X_{i2} - \hat{\mu}_\omega)^2]\right)$$

and

$$-2\ln(\Lambda) = 2n\ln\left(\frac{\hat{\sigma}_\omega^2}{\hat{\sigma}_1\hat{\sigma}_2}\right)\,.$$

Using the transformation

$$\zeta(\theta) = \begin{pmatrix} \mu_1 - \mu_2 \\ \sigma_1^2 - \sigma_2^2 \\ \mu_2 \\ \sigma_2^2 \end{pmatrix} \text{ for } \theta = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \sigma_1^2 \\ \sigma_2^2 \end{pmatrix},$$

the information matrix is

$$\mathcal{I}(\zeta) = \frac{\partial\theta^T}{\partial\zeta}\mathcal{I}(\theta)\frac{\partial\theta}{\partial\zeta^T}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1/\sigma_1^2 & 0 & 0 & 0 \\ 0 & 1/\sigma_2^2 & 0 & 0 \\ 0 & 0 & 1/(2\sigma_1^4) & 0 \\ 0 & 0 & 0 & 1/(2\sigma_2^4) \end{pmatrix} \begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1/\sigma_1^2 & 0 & 1/\sigma_1^2 & 0 \\ 0 & 1/(2\sigma_1^4) & 0 & 1/(2\sigma_1^4) \\ 1/\sigma_1^2 & 0 & 1/\sigma_1^2 + 1/\sigma_2^2 & 0 \\ 0 & 1/(2\sigma_1^4) & 0 & 1/(2\sigma_1^4) + 1/(2\sigma_2^4) \end{pmatrix}\,.$$

With $\sigma_1^2 = \sigma_2^2$ we have

$$\mathcal{I}(\zeta^*) = \begin{pmatrix} 1/\sigma_2^2 & 0 & 1/\sigma_2^2 & 0 \\ 0 & 1/(2\sigma_2^4) & 0 & 1/(2\sigma_2^4) \\ 1/\sigma_2^2 & 0 & 2/\sigma_2^2 & 0 \\ 0 & 1/(2\sigma_2^2) & 0 & 1/\sigma_2^4 \end{pmatrix}\,.$$

$$\mathcal{I}^{-1}(\zeta^*) = \begin{pmatrix} 2\sigma_2^2 & 0 & -\sigma_2^2 & 0 \\ 0 & 4\sigma_2^4 & 0 & -2\sigma_2^4 \\ -\sigma_2^2 & 0 & \sigma_2^2 & 0 \\ 0 & -2\sigma_2^4 & 0 & 2\sigma_2^4 \end{pmatrix}$$

and

$$\bar{C}_{11}(\zeta^*) = \begin{pmatrix} 1/(2\sigma_2^4) & 0 \\ 0 & 1/(4\sigma_2^4) \end{pmatrix}.$$

Then

$$-2\ln(\Lambda) \xrightarrow{L} \chi_2^2(\lambda^2) \text{ where } \lambda^2 = \frac{\delta_1^2}{2\sigma_2^2} + \frac{\delta_2^2}{4\sigma_2^4}$$

and $\mu_1 - \mu_2 = \delta_1/\sqrt{n}, \quad \sigma_1^2 - \sigma_2^2 = \delta_2/\sqrt{n}$.

The result can be extended to the problem of several independent samples

$$X_{ij} \text{ for } i = 1, 2, \ldots, K, \quad j = 1, 2, \ldots, n_i$$

where $f_i(x_{ij}|\theta)$ is the density for X_{ij}, the same for the ith sample for $j = 1, 2, \ldots, n_i$ and all X_{ij} independent.
We assume that assumptions A,B,C,D hold and that

$$\mathcal{I}(\theta) = \sum_{i=1}^{K} \rho_i E_\theta \left(\frac{\partial \ln(f_i)}{\partial \theta} \frac{\partial \ln(f_i)}{\partial \theta^T} \right) = -\sum_{i=1}^{n} \rho_i E_\theta \left(\frac{\partial^2 \ln(f_i)}{\partial \theta \partial \theta^T} \right)$$

where $\rho_i = n_i/N$, $N = \sum_{i=1}^{K} n_i$. Then the result is as given in theorem 12.5.

12.4 Conditional Generalized Likelihood Ratio Test

To obtain a test with an exact null distribution, if a sufficient statistic exists under the hypothesis, we can condition on it to obtain a distribution that is free of unknown parameters. In many cases, the properties of the conditional LR test are asymptotically the same as the optimal properties of the generalized LR test. Bahadur and Raghavachari[7] discuss efficies for the conditional and unconditional tests.

[7]Bahadur, R.R. and Raghavachari (1972) Some Asymptotic Properties of Likelihood Ratios on General Sample Spaces. *Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability.* Berkeley and Los Angeles. *University of California Press* **1** *129-152.*

For an example, Let $\mathbf{X} = (X_{11}, X_{12}, \ldots, X_{rc})$ and

$$P(\mathbf{X} = \mathbf{x}) = \frac{n!}{x_{11}!x_{12}!\cdots x_{rc}!} p_{11}^{x_{11}} p_{12}^{x_{12}} \cdots p_{rc}^{x_{rc}}$$

$$\text{where } \sum_{i=1}^{r}\sum_{j=1}^{c} p_{ij} = 1 \text{ and } \sum_{i=1}^{r}\sum_{j=1}^{c} x_{ij} = n \ .$$

For testing $H : p_{ij} = p_{i+}p_{+j}$ where $p_{i+} = \sum_{j=1}^{c} p_{ij}$ and $p_{+j} = \sum_{i=1}^{c} p_{ij}$ for all i, j versus $A : p_{ij} \neq p_{i+}p_{+j}$ for some i, j the sufficient statistics under H are $\{X_{i+} : i = 1, 2, \ldots, r\}$ and $\{X_{+j} : j = 1, 2, \ldots, c\}$ where $X_{i+} = \sum_{j=1}^{c} X_{ij}$ and $X_{+j} = \sum_{i=1}^{r} X_{ij}$.

The conditional distribution

$$P_H(\mathbf{X} = \mathbf{x})|X_{i+} = x_{i+}, X_{+j} = x_{+j}, i = 1, 2, \ldots, r,\ j = 1, 2, \ldots, c)$$

$$= \frac{\prod_{i=1}^{r} (x_{i+}!/(x_{i1}!x_{i2}!\cdots x_{ic}!))}{n!/(x_{+1}!x_{+2}!\cdots x_{+c}!)} \tag{12.19}$$

does not depend on p_{i+} or p_{+j} under H.

The generalized likelihood ratio statistic is

$$-2\ln(\Lambda) = 2\left[\sum_{i=1}^{r}\sum_{j=1}^{c} X_{ij} \ln\left(nX_{ij}/(X_{i+}X_{+j})\right)\right]. \tag{12.20}$$

The P-value of this test which rejects for large values of $-2\ln(\Lambda)$ conditionally given X_{i+}, X_{+j} can be obtained by enumerating all $r \times c$ matrices that have row margins X_{i+} and column margins X_{+j}. For each such matrix we calculate the statistic (12.20) and add the conditional probability (12.19) if the statistic is equal or greater than the observed value of $-2\ln(\Lambda)$.

This is a straightforward but inefficient way to do the calculation. The C++ program **rxcIndep.cpp** in **Appendix F** calculates exact P-values for small counts. For the UNIX system we compile the program (using gnu C++) with the with the command **g++ -o rxcIndep rxcIndep.cpp**. Using the file **rxc.dat**, with r=3, and c=4, we execute it with the command

rxcIndep rxc.dat

and get the following output:

Table 12.1: Test Data **rxc.dat** for rxcIndep Program

3	4		
10	9	7	3
8	4	6	7
0	2	12	9

```
Likelihood ratio test conditional on the margins X[i,+],X[+,j]
for an rxc table X[i,j] i=1,2,...,r, j=1,2,...,c with multinomial
dist. testing independence H: p[i,j]=p[i,+]p[+,j] for all i,j.
The program generates all non negative integer component matrices u
with margins equal to X[i,+],X[+,j]. The P-value is computed by adding
up P(u|X[i,+],X[+,j]) for each matrix u with T(u)>=T(X) where X is
the data matrix & T is equivalent to the LR statistic -2ln(lambda).
Data Matrix X
|   10    9    7    3  |29
|    8    4    6    7  |25
|    0    2   12    9  |23
|_______________________|
    18   15   25   19  |77
-2ln(lambda)=24.8408

Starting Matrix
|   18   11    0    0  |29
|    0    4   21    0  |25
|    0    0    4   19  |23
|_______________________|
    18   15   25   19  |77
Ending Matrix
|    0    0   10   19  |29
|    0   10   15    0  |25
|   18    5    0    0  |23
|_______________________|
    18   15   25   19  |77

P-value: P[-2ln(lambda)>=24.8408|X[i,+],X[+,j]]=0.000740365
```

```
Total matrices enumerated=3084350.
```

We note the large number of matrices enumerated, even for a fairly small contingency table. An improved algorithm is given by Seung-Ho Kang [8] that covers larger cases. However, the chi-square approximation

$$P_H(-2\ln(\Lambda) > x | x_{i+}, x_{+j}) \doteq P(\chi^2_{(r-1)(c-1)}(0) > x)$$

is used for cases that are too large for the exact calculation.

For another example, consider the multinomial genetic model

$$P(X_{ijk} = x_{ijk}\ 1 \le i \le r,\ 1 \le j \le k \le m) = n! \prod_{i=1}^{r} \prod_{j=1}^{m} \prod_{k=j}^{m} \frac{p_{ijk}^{x_{ijk}}}{x_{ijk}!}$$

for integer $1 \le i \le r,\ 1 \le j \le k \le m$. Here the index i corresponds to an attribute B_i and the indices j, k correspond to genotypes $A_j A_k$ of a diploid genetic system with m different genes in one locus.

The hypothesis for testing independence of attributes and genotype as well as if the genotype follows the Hardy-Weinberg equilibrium law is

$$H:\ p_{ijk} = \gamma_i \rho_j \rho_k (2 - \delta_{jk}) \text{ for all } i, j, k$$

where $\sum_{i=1}^{r} \gamma_i = 1$, $\sum_{j=1}^{m} \rho_j = 1$, $\delta_{jk} = 1$ if $j = k$, and $\delta_{jk} = 0$ if $j \ne k$.

Under the hypothesis

$$P_H(X_{ijk} = x_{ijk} \text{ for all } i, j, k) = \frac{n! 2^{x^*_{+++}}}{\prod_{i=1}^{r} \prod_{j=1}^{m} \prod_{k=j}^{m} x_{ijk}!} \left(\prod_{i=1}^{r} \gamma_i^{x_{i++}} \right) \left(\prod_{j=1}^{m} \rho_j^{x^*_{+j+}} \right)$$

where

$$x_{+jk} = \sum_{i=1}^{r} x_{ijk}, \quad x^*_{+++} = \sum_{j=1}^{m-1} \sum_{k=j+1}^{m} x_{+jk},$$

and for $i = 1, 2, \ldots, r$, $j = 1, 2, \ldots, m$

$$X_{i++} = \sum_{j=1}^{m} \sum_{k=j}^{m} X_{ijk}, \quad X^*_{+j+} = \sum_{t=1}^{j} X_{+tj} + \sum_{k=j}^{m} X_{+jk},$$

[8] Kang, Seung-Ho (1997). *The Conditional Likelihood Ratio Test of Independence in Two-Way Contingency Tables.* University of Wisconsin, Madison Ph.D. Thesis (Statistics).

are the sufficient statistics for $\{\gamma_i\}$, $\{\rho_j\}$ under H.

We have,

$$P_H(X_{i++} = x_{i++} : 1 \le i \le r) = n! \prod_{i=1}^{r} \frac{\gamma_i^{x_{i++}}}{x_{i++}!}$$

$$P_H(X^*_{+j+} = x^*_{+j+} : 1 \le j \le m) = (2n)! \prod_{j=1}^{m} \frac{\rho_j^{x^*_{+j+}}}{x^*_{+j+}!}$$

with $\{X_{i++}\ i = 1, 2, \ldots, r\}\ : \mathcal{M}(n, (\gamma_1.\gamma_2, \ldots, \gamma_m))$, and $\{X^*_{+j+}\ j = 1, 2, \ldots, m\}\ :$ $\mathcal{M}(2n, (\rho_1, \rho_2, \ldots, \rho_m))$ independent under H.

The generalized likelihood ratio statistic $-2\ln(\Lambda) =$

$$2\left[\sum_{i=1}^{r}\sum_{j=1}^{m}\sum_{k=1}^{j} X_{ijk} \ln\left(\frac{X_{ijk}}{n}\right) - \sum_{i=1}^{r} X_{i++} \ln\left(\frac{X_{i++}}{n}\right) - \sum_{j=1}^{m} X^*_{+j+} \ln\left(\frac{X^*_{+j+}}{2n}\right) - X^*_{+++} \ln(2)\right]$$

and

$$P_H(X_{ijk} = x_{ijk} | x_{i++}, x^*_{+j+} : \forall i, j, k) = \frac{(\prod_{i=1}^{r} x_{i++}!)(\prod_{j=1}^{m} x^*_{+j+}!)2^{x^*_{+++}}}{(\prod_{i=1}^{r}\prod_{j=1}^{m}\prod_{k=j}^{m} x_{ijk}!)(2n)!}\ .$$

The P-value of the conditional generalized likelihood ratio test could be obtained by enumerating all possible tables of $\{X_{ijk}\}$ which have values $\{x_{i++}\}$, $\{x^*_{+j+}\}$ the same as the data and adding up the tables probability $P_H(X_{ijk} = x_{ijk} | x_{i++}, x^*_{+j+} : \forall i, j, k)$ if its value of $-2\ln(\Lambda)$ is greater or equal the data's statistic (a difficult task).

12.5 Problems

1. Let $X_1, X_2, \ldots, X_n$ be independent Uniform$(0, \theta)$. Derive the UMP test of $H :\ \theta = \theta_0$.

2. Let $X_1, X_2, \ldots, X_m$ be independent $\mathcal{N}(\mu, \sigma^2)$ and $Y_1, Y_2, \ldots, Y_n$ be independent $\mathcal{N}(\eta, \sigma^2)$ where σ^2 is known. Derive the UMP test of $H :\ \mu = \eta$ versus $A :\ \mu > \eta$.

3. Let $X_1, X_2, \ldots, X_n$ be independent Poisson(θ) and $Y_1, Y_2, \ldots, Y_n$ independent Poisson(η). Derive the UMP unbiased test of $H :\ \theta = \eta$ versus $A :\ \theta > \eta$. Is this test also UMP?

4. Let $\{X_{ijk} : i, j = 1, 2\}$ be independent for $k = 1, 2$ with

$$P(X_{ijk} = x_{ijk} : i, j = 1, 2) = n_k! \prod_{i=1}^{2} \prod_{j=1}^{2} \frac{p_{ijk}^{x_{ijk}}}{x_{ijk}!}$$

where $x_{ijk} \in \{0, 1, \ldots, n_k\}$, $\sum_{i=1}^{2} \sum_{j=1}^{2} x_{ijk} = n_k$ $\sum_{i=1}^{2} \sum_{j=1}^{2} p_{ijk} = 1$, $0 \leq p_{ijk} \leq 1$. Derive the UMP unbiased test of $H: \ p_{111} = p_{112}$ versus $A: \ p_{111} > p_{112}$.

5. Let $\mathbf{X} = \{X_{ij} : i, j = 1, 2, \ldots, m\}$ have the multinomial joint distribution $\mathcal{M}(n, \{p_{ij} : i, j = 1, 2, \ \ldots, m\})$ given by

$$P(\mathbf{X} = \mathbf{x}) = n! \prod_{i=1}^{m} \prod_{j=1}^{m} \frac{p_{ij}^{x_{ij}}}{x_{ij}!}$$

where integer $x_{ij} \in \{0, 1, \ldots, n\}$, $\sum_{i=1}^{m} \sum_{j=1}^{m} x_{ij} = n$, $0 \leq p_{ij} \leq 1$,and $\sum_{i=1}^{m} \sum_{j=1}^{m} p_{ij} = 1$. Consider the hypothesis and alternative

$$H: \ p_{ij} = \rho_1 \rho_j \text{ for all } i, j = 1, 2, \ldots m \text{ and } A: \ p_{ij} \neq \rho_i \rho_j \text{ for some } i, j$$

where $0 \leq \rho_i \leq 1$ and $\sum_{i=1}^{m} \rho_i = 1$.
Derive the generalized likelihood ratio statistic $-2\ln(\Lambda)$. Give the conditional generalized likelihood ratio statistic for testing H and discuss how to calculate its exact P-value.

6. Let X_i, $i = 1, 2, \ldots, n$ be independent $\mathcal{N}(a_i \mu, b_i^2 \sigma^2)$ where (a_i, b_i^2) are known, (μ, σ^2) unknown. Derive the UMP unbiased test of $H: \ \mu = \mu_0$ versus $A: \ \mu > \mu_0$ where μ_0 is known.

7. Let

$$X_{jk} = \mu + a_j + \varepsilon_{jk} \text{ for } j = 1, 2, \ldots, J, \ k = 1, 2, \ldots, K$$

where a_j are independent $\mathcal{N}(0, \sigma_a^2)$ and ε_{jk} are independent $\mathcal{N}(0, \sigma_e^2)$. Derive the UMP unbiased test of $H: \ \sigma_a^2 = 0$ versus $A: \ \sigma_a^2 > 0$.

Chapter 13

Interval Estimation

13.1 Confidence Intervals

We define a comfidence interval for a parameter θ with confidence probability $1-\alpha$ based on the observations $\mathbf{X}$ with distribution in $\mathcal{P} = \{p_\theta(\mathbf{x}) : \theta \in \Theta\}$ as a pair of random variables $(L(\mathbf{X}), U(\mathbf{X}))$ that satisfy

$$P_\theta(L(\mathbf{X}) \leq \theta, \text{ and } U(\mathbf{X}) \geq \theta) \geq 1-\alpha \text{ for all } \theta \in \Theta \ .$$

For example, let $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ where $X_i : \mathcal{N}(\theta, 1)$ are independent. Then a $1-\alpha$ confidence interval for θ is

$$(L(\mathbf{X}), U(\mathbf{X})) = (\bar{X} - \frac{z_{\alpha/2}}{\sqrt{n}}, \bar{X} + \frac{z_{\alpha/2}}{\sqrt{n}})$$

where, for the standard normal cdf, $\Phi(z_{\alpha/2}) = 1-\alpha/2$. and $\bar{X} = \sum_{i=1}^n X_i/n$. This follows from $P_\theta(L(\mathbf{X}) \leq \theta, \text{ and } U(\mathbf{X}) \geq \theta) =$

$$P(-z_{\alpha/2} \leq \sqrt{n}(\bar{X} - \theta) \leq z_{\alpha/2}) = \Phi(z_{\alpha/2}) - \Phi(-z_{\alpha/2}) = 1-\alpha$$

for all $\theta \in (-\infty, \infty) = \Theta$.

More generally, we say that the random set $\mathcal{S}(\mathbf{X})$ is a $1-\alpha$ confidence set for θ if

$$P_\theta(\theta \in \mathcal{S}(\mathbf{X})) = 1-\alpha \text{ for all } \theta \in \Theta$$

(the random set $\mathcal{S}(\mathbf{X})$ covers the fixed parameter θ with probability $1-\alpha$).

We can construct confidence sets from tests of hypotheses. Let $\mathcal{A}(\theta_0)$ be the acceptance region for testing the hypothesis $H_{\theta_0} : \ \theta = \theta_0$ versus the

alternative A_{θ_0} where

$$P_{\theta_0}(\mathbf{X} \in \mathcal{A}(\theta_0)) = 1 - \alpha \text{ for every } \theta_0 \in \Theta \ .$$

If we define $\mathcal{S}(\mathbf{X}) = \{\theta : \ \mathbf{X} \in \mathcal{A}(\theta), \theta \in \Theta\}$ then $\mathcal{S}(\mathbf{X})$ is a $1 - \alpha$ confidence set for θ since

$$P_\theta(\theta \in \mathcal{S}(\mathbf{X})) = P_\theta(\mathbf{X} \in \mathcal{A}(\theta)) = 1 - \alpha \ .$$

As an example, consider the t-test for testing $H_{\mu_0} : \mu = \mu_0$ versus the alternative $A_{\mu_0} : \ \mu \neq \mu_0$ based on $X_1, X_2, \ldots, X_n$ independent $\mathcal{N}(\mu, \sigma^2)$. Then the acceptance region for the UMP unbiased test is

$$\mathcal{A}(\mu_0) = \{(X_1, X_2, \ldots, X_n) : \ -t_{\alpha/2,n-1} \leq \frac{\sqrt{n}(\bar{X} - \mu_0)}{S} \leq t_{\alpha/2,n-1}\}$$

where $\bar{X} = \sum_{i=1}^n X_i/n$, $S = [\sum_{i=1}^n (X_i - \bar{X})^2/(n-1)]^{1/2}$ and the corresponding confidence set is

$$\mathcal{S}(X_1, X_2, \ldots, X_n) = \{\mu : \ \bar{X} - t_{\alpha/2,n-1}\frac{S}{\sqrt{n}} \leq \mu \leq \bar{X} + t_{\alpha/2,n-1}\frac{S}{\sqrt{n}}\} \ .$$

For confidence sets generated from tests with optimality properties, there is a corresponding optimality property. For example, if the confidence set is generated from a UMP test, then the probability that the confidence set covers false values of θ is a minimum since

$$P_\theta(\theta_0 \in \mathcal{S}(\mathbf{X})) = P_\theta(\mathbf{X} \in \mathcal{A}(\theta_0)) \text{ is a minimum for } \theta \in A_{\theta_0} \ .$$

For confidence sets generated from UMP unbiased tests, we have

$$P_\theta(\theta_0 \in \mathcal{S}(\mathbf{X})) = P_\theta(\mathbf{X} \in \mathcal{A}(\theta_0)) \leq 1 - \alpha \text{ for } \theta \in A_{\theta_0}$$

and the probability of covering a false parameter value is smaller than the probability of covering the true parameter value.

The confidence interval for σ^2 with $X_1, X_2, \ldots, X_n$ independent $\mathcal{N}(\mu, \sigma^2)$ corresponding to the UMP unbiased test of $H : \ \sigma^2 = \sigma_0^2$ versus $A : \sigma^2 \neq \sigma_0^2$ has the acceptance region

$$\mathcal{A}(\sigma_0^2) = \{(X_1, X_2, \ldots, X_n) : \ C_1 \leq \sum_{i=1}^n (X_i - \bar{X})^2/\sigma_0^2 \leq C_2\}$$

and associated unbiased confidence interval

$$\mathcal{S}(\mathbf{X}) = \{\sigma^2 : \frac{\sum_{i=1}^n (X_i - \bar{X})^2}{C_2} \leq \sigma^2 \leq \frac{\sum_{i=1}^n (X_i - \bar{X})^2}{C_1}\} .$$

Here $U = \sum_{i=1}^n (X_i - \bar{X})^2/\sigma^2$ has the chi-square distribution with degrees of freedom parameter $\nu = n - 1$ and critical values (C_1, C_2) satisfy equations

$$P(C_1 \leq U \leq C_2) = \int_{C_1}^{C_2} f_{\chi^2_\nu}(u)du = 1 - \alpha \tag{13.1}$$

$$\int_{C_1}^{C_2} f_{\chi^2_{\nu+2}}(u)du = 1 - \alpha. \tag{13.2}$$

To solve for (C_1, C_2), we integrate equation (13.2) by parts and obtain the equation

$$C_1^\nu e^{-C_1} = C_2^\nu e^{-C_2} .$$

Writing $r = C_1/C_2$ this can be written as

$$C_2 = \nu \frac{\ln(r)}{(r-1)} .$$

We iterate on $r \in (0, 1)$ by means of a half interval search with lower bound $\underline{r} = 0$ and upper bound $\overline{r} = 1$ and starting values $C_2 = \nu \ln(r)/(r - 1))$, $C_1 = rC_2$ for $r = 1/2$. The C++ program **OneVar.cpp** in **Appendix G** searches until equation (13.1) is satisfied to within $\varepsilon = 10^{-10}$. m For the case of μ known, the program uses $U = \sum_{i=1}^n (X_i - \mu)^2/\sigma^2$ and degrees of freedom parameter $\nu = n$.

For $X_1, X_2, \ldots, X_m$ independent $\mathcal{N}(\mu, \sigma^2)$ and $Y_1, Y_2, \ldots, Y_n$ independent $\mathcal{N}(\eta, \sigma^2)$ the UMP unbiased test of $H : \ \delta = \mu - \eta = \delta_0$ versus $A : \ \delta \neq 0$ with σ^2 unknown has acceptance region for type I error α given by

$$\mathcal{A}(\delta_0) = \{\mathbf{X}, \mathbf{Y} : -t_{\nu\alpha/2} \leq \frac{(\bar{X} - \bar{Y} - \delta_0)}{S\sqrt{(1/m) + (1/n)}} \leq -t_{\nu\alpha/2}\}$$

and the corresponding $1 - \alpha$ probability confidence set is $\mathcal{S}(\mathbf{X}, \mathbf{Y}) =$

$$\{\delta : \ (\bar{X} - \bar{Y}) - t_{\nu\alpha/2} S\sqrt{(1/m) + (1/n)} \leq \delta \leq (\bar{X} - \bar{Y}) + t_{\nu\alpha/2} S\sqrt{(1/m) + (1/n)}\} .$$

Here $T = (\bar{X} - \bar{Y} - \delta)/(S\sqrt{(1/m) + (1/n)})$ has the Student t distribution, $t_{\nu,\alpha/2}$ is the upper $\alpha/2$, percentage point of the t distribution

$(P(T > t_{\nu,\alpha/2}) = \alpha/2)$, the degrees of freedom parameter is $\nu = m + n - 2$, and

$$S^2 = \sum_{i=1}^{m}(X_i - \bar{X})^2 + \sum_{j=1}^{n}(Y_j - \bar{Y})^2, \quad S = \sqrt{S^2}.$$

For $X_1, X_2, \ldots, X_m$ independent $\mathcal{N}(\mu, \sigma^2)$ and $Y_1, Y_2, \ldots, Y_n$ independent $\mathcal{N}(\eta, \tau^2)$ the UMP unbiased test of $\rho = \sigma^2/\tau^2 = \rho_0$ versus $A: \ \rho \neq \rho_0$ has type I error α acceptance region given by

$$\mathcal{A}(\rho_0) = \{\mathbf{X}, \mathbf{Y} : C_1 \leq \frac{S_X^2}{S_X^2 + \rho_0 S_Y^2} \leq C_2\}$$

and $1 - \alpha$ probability confidence interval

$$\mathcal{S}(\mathbf{X}, \mathbf{Y}) = \{\rho : \frac{S_X^2(1 - C_2)}{S_Y^2 C_2} \leq \rho \leq \frac{S_X^2(1 - C_1)}{S_y^2 C_1}\} \ .$$

Here $U = S_X^2/(S_X^2 + \rho S_y^2)$ has the incomplete beta distribution $I_u(\nu_1/2, \nu_2/2)$ with degrees of freedom $(\nu_1, \nu_2) = (m - 1, n - 1)$,

$$S_X^2 = \sum_{i=1}^{m}(X_i - \bar{X})^2, \quad S_Y^2 = \sum_{j=1}^{n}(Y_j - \bar{Y})^2,$$

and the critical values (C_1, C_2), where $0 < C_1 < C_2 < 1$ satisfy

$$\int_{C_1}^{C_2} \frac{\Gamma((\nu_1 + \nu_2)/2)}{\Gamma(\nu_1/2)\Gamma(\nu_2/2)} u^{\nu_1/2}(1 - u)^{\nu_2/2} du = 1 - \alpha \tag{13.3}$$

and

$$\int_{C_1}^{C_2} \frac{\Gamma((\nu_1 + 2 + \nu_2)/2)}{\Gamma((\nu_1 + 2)/2)\Gamma(\nu_2/2)} u^{(\nu_1+2)/2}(1 - u)^{\nu_2/2} du = 1 - \alpha \tag{13.4}$$

Manipulating equation (13.4) we reduce it to

$$\nu_1 \ln(C_1) + \nu_2 \ln(1 - C_1) = \nu_1 \ln(C_2) + \nu_2 \ln(1 - C_2) \ .$$

If we write $r = \nu_1/\nu_2$ and $F1 = C_1/(r(1 - C_1)$, $F2 = C_2/(r(1 - C_2)$ then the $1 - \alpha$ confidence interval is

$$\{\frac{S_X^2/(m - 1)}{F2 S_Y^2/(n - 1)} \leq \rho \leq \frac{S_X^2/(m - 1)}{F1 S_Y^2/(n - 1)}\}$$

in terms of critical values $(F1, F2)$ for the F_{ν_1,ν_2} distribution of

$$\mathcal{F} = \frac{S_X^2/(m-1)}{\rho S_Y^2/(n-1)} \ .$$

The C++ program **TwoVar.cpp** in **Appendix H** calculates the value of the confidence interval iterating on C_1 and C_2 to satisfy the equations. For the case where (μ, ν) is known we input $(\nu_1, \nu_2) = (m, n)$ for the degrees of freedom parameter and

$$S_X^2 = \sum_{i=1}^{m}(X_i - \mu)^2, \quad S_Y^2 = \sum_{j=1}^{n}(Y_j - \nu)^2$$

for the sums of squares.

Often, because of simplicity, **equal tail** confidence intervals are used instead of UMP unbiased condidence intervals. For example, we use

$$\mathcal{S}(\mathbf{X}) = \{\sigma^2 : \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{C_2} \leq \sigma^2 \leq \frac{\sum_{i=1}^{n}(X_i - \bar{X})^2}{C_1}\}$$

where

$$\int_0^{C_1} f_{\chi_\nu^2}(u)du = \alpha/2 = \int_{C_2}^{\infty} f_{\chi_\nu^2}(u)du$$

for a confidence interval for σ^2 when $X_1, X_2, \ldots, X_n$ are independent $\mathcal{N}(\mu, \sigma^2)$.

For two independent samples $X_1, X_2, \ldots, X_m : \mathcal{N}(\mu, \sigma^2)$, and $Y_1, Y_2, \ldots, Y_n : \mathcal{N}(\nu, \tau^2)$, with $\rho = \sigma^2/\tau^2$, we use

$$\mathcal{S}(\mathbf{X}, \mathbf{Y}) = \{\rho : \frac{S_X^2/(m-1)}{F_2 S_Y^2/(n-1)} \leq \rho \leq \frac{S_X^2/(m-1)}{F_1 S_y^2/(n-1)}\}$$

where, using the $\mathcal{F}_{\nu_1,\nu_2}$ distribution,

$$\int_0^{F_1} f_{\mathcal{F}_{\nu_1,\nu_2}}(v)dv = \alpha/2 = \int_{F_2}^{\infty} f_{\mathcal{F}_{\nu_1,\nu_2}}(v)dv \ .$$

For discrete distributions, the equal tail test is often modified to an approximate conservative equal tail test. Consider the acceptance interval with probability at least $1-\alpha$ for a parameter θ in an interval based on the statistic $T(\mathbf{X})$ with monotone likelihood given by

$$\mathcal{A}(\theta_0) = \{\mathbf{X} : C_1 < T(\mathbf{X}) < C_2\}$$

with C_1, C_2 satisfying

$$\alpha_1 = \sum_{T(\mathbf{x}) \le C_1} P_{\theta_0}[T(\mathbf{X}) = T(\mathbf{x})] \le \alpha/2, \quad \alpha_2 = \sum_{T(\mathbf{x}) \ge C_2} P_{\theta_0}[T(\mathbf{X}) = T(\mathbf{x})] \le \alpha/2 \ .$$

We choose α_1, α_2 as close as possible but les than or equal to $\alpha/2$ and the acceptance probability is $1 - \alpha_1 - \alpha_2 \ge 1 - \alpha$. The conservative confidence interval with confidence coefficient at least $1 - \alpha$ for an observed value $\mathbf{x}$ is then often of the form

$$\mathcal{S}(\mathbf{x}) = \{\theta : \mathbf{X} \in \mathcal{A}(\theta)\} = \{\theta : \theta_L(\mathbf{x}) \le \theta \le \theta_U(\mathbf{x})\}$$

where $\theta_L(\mathbf{x}), \theta_U(\mathbf{x})$ satisfy

$$\sum_{T(\mathbf{y}) \ge T(\mathbf{x})} P_{\theta_L}[T(\mathbf{X}) = T(\mathbf{y})] = \alpha/2, \quad \sum_{T(\mathbf{y}) \le T(\mathbf{x})} P_{\theta_U}[T(\mathbf{X}) = T(\mathbf{y})] = \alpha/2 \ .$$

We define the confidence coefficient as the infimum over the θ parameter space of the probability that $\mathcal{S}(\mathbf{X})$ covers θ.

As an example, let X have a binomial(n, p) distribution. The equal tail confidence interval with confidence coefficient $1 - \alpha$ for an observed value x satisfies

$$\mathcal{S}(x) = \{p : p_L(x) \le p \le p_U(x)\}$$

where

$$\sum_{y=x}^{n} \binom{n}{y} p_L^y (1 - p_L)^{n-y} = \alpha/2, \quad \sum_{y=0}^{x} \binom{n}{y} p_U^y (1 - p_U)^{n-y} = \alpha/2 \ .$$

The solutions, $p_L(X), p_U(x)$, can be obtained from the inverse of the incomplete beta function by solving

$$\int_0^{p_L} \frac{\Gamma(n+1)}{\Gamma(x)\Gamma(n-x+1)} u^{x-1}(1-u)^{n-x} du = I_{p_L}(x, n-x+1) = \alpha/2,$$

$$I_{p_U}(x+1, n-x) = 1 - \alpha/2$$

using the relation between the incomplete beta function and the binomial distribution (chapter 3).

For X distributed as Poisson(λ), the equal tail confidence interval for λ with confidence coefficient $1 - \alpha$ is obtained similarly

$$\mathcal{S}(x) = \{\lambda : \lambda_L(x) \le \lambda \le \lambda_U(x)\}$$

where

$$\sum_{y=x}^{\infty} \frac{\lambda_L^y}{y!} e^{-\lambda_L} = \alpha/2, \quad \sum_{y=0}^{x} \frac{\lambda_U^y}{y!} e^{-\lambda_U} = 1 - \alpha/2 \ .$$

Using the relation of the Poisson cdf and the incomplete gamma function (chapter 3), we can solve for $\lambda_L(x), \lambda_U(x)$ from

$$\int_0^{\lambda_L} \frac{u^{x-1}e^{-u}}{\Gamma(x)} du = G(x, \lambda_L) = \alpha/2, \quad G(x+1, \lambda_U) = 1 - \alpha/2 \ .$$

13.2 Bayesian Intervals

If $\mathbf{X}$ has a distribution $P(\mathbf{x}|\theta)$ for $\theta \in \Theta$ with a prior distribution $\Lambda(\theta)$ over the parameter space Θ, we define a Bayesian confidence set or γ probability *credible region* $\mathcal{S}(\mathbf{x})$ as a set that satisfies the posterior probability

$$P[\theta \in \mathcal{S}(\mathbf{x})|\mathbf{X} = \mathbf{x}) \geq \gamma$$

for all $\mathbf{x}$.

For example, let X have a binomial(n, p) distribution, and consider the prior density

$$\lambda(p) = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)} p^{\alpha-1}(1-p)^{\beta-1} \text{ for } 0 < p < 1 \ .$$

Then a γ probability cedible interval for p is

$$\mathcal{S}(x) = \{p : p_L(x) < p < p_U(x)\}$$

where α, β, and γ are given, and $p_L(x), p_U(x)$ satisfy the posterior probability

$$\int_{p_L(x)}^{p_U(x)} \frac{\Gamma(n+\alpha+\beta)}{\Gamma(x+\alpha)\Gamma(n-x+\beta)} p^{x+\alpha-1}(1-p)^{n-x+\beta-1} dp = \gamma \ .$$

Usually, $p_L(x), p_U(x)$ are chosen to make the interval as short as possible for the specified value of γ forming the highest (posterior) probability density (HPD) region.

13.3 Problems

1. Let $X_1, X_2, \ldots, X_n$ be independent with gamma density

$$f)X_i(x_i) = \frac{x_i^{\alpha-1}e^{-x_i/\sigma}}{\sigma^\alpha\Gamma(\alpha)} \text{ for } 0 < x_i < \infty$$

where (α, σ) are unknown.
Derive the UMPU confidence interval for σ.

2. Let $(X_{11}, X_{12}, X_{21}, X_{22})$ have the multinomial($n, p_{11}, p_{12}, p_{21}, p_{22}$) distribution, $p_{11} + p_{12} + p_{21} + p_{22} = 1$. Construct the UMPU confidence interval for p_{11}.

3. Let X, Y have joint density

$$P(X = x, Y = y) = \frac{(x + y + r - 1)!}{x!y!(r - 1)!} p_1^x p_2^y p_3^r \text{ for } x, y = 0, 1, 2, \ldots, \infty$$

where r is known, (p_1, p_2) unknown, $p_1 + p_2 + p_3 = 1$, $0 \le p_1, p_2 \le 1$. Construct the UMPU confidence interval for p_1.

4. Let X, Y be independent with Gamma (α, σ) and Gamma (β, τ) densities respectively. Derive the equal tail confidence interval for $\rho = \sigma/\tau$.

5. Let

$$\mathbf{Y}^{n\times 1} = \mathbf{X}^{n\times p}\beta^{p\times 1} + \varepsilon^{n\times 1}$$

where ε is multivariate normal $\mathcal{N}_n(\mathbf{0}, \sigma^2\mathbf{I}_n)$ for the $n \times n$ identity matrix $\mathbf{I}_n$ with β and σ unknown. Here $n > p \ge r$ where r is the rank of $\mathbf{X}$. Construct the UMPU confidence interval for

$$\psi = \sum_{i=1}^{p} a_i\beta_i$$

where $(a_1, a_2, \ldots, a_p)$ are known. Also give the UMPU confidence interval for σ^2.

6. Let X have Poisson(λ) density. For the conjugate Gamma prior

$$f_\Lambda(\lambda) = \frac{\lambda^\alpha e^{-\lambda/\sigma}}{\sigma^\alpha\Gamma(\alpha)} \text{ for } 0 < \lambda < \infty$$

where (α, σ) are known, give the HPD Bayesian credible interval for λ.

Chapter 14

The General Linear Hypothesis

We consider the model

$$Y_i = \sum_{j=1}^{p} x_{ij}\beta_j + \varepsilon_i \text{ for } i = 1, 2, \ldots, n$$

where ε_i are indepndent $\mathcal{N}(0, \sigma^2)$. In matrix notation,

$$\mathbf{Y}^{n\times 1} = \mathbf{X}^{n\times p}\boldsymbol{\beta}^{p\times 1} + \boldsymbol{\varepsilon}^{n\times 1}$$

where $\boldsymbol{\varepsilon}$ is multivariate normal $\mathcal{N}_n(\mathbf{0}, \sigma^2\mathbf{I}_n)$ for the $n \times n$ identity matrix $\mathbf{I}_n$ with β and σ unknown and $n > p \geq r$, with r the rank of $\mathbf{X}$.

14.1 Least Square, M.L.,and UMVU Estimates of β

The least square estimates of $\boldsymbol{\beta}$ are defined to be a solution to the problem of minimizing

$$\mathcal{S}^2(\boldsymbol{\beta}) = \sum_{i=1}^{n}(Y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2$$

with respect to $\boldsymbol{\beta}$. The solution, which need not be unique, satisfies the normal equations

$$\frac{\partial \mathcal{S}(\boldsymbol{\beta})}{\partial \boldsymbol{\beta}} = \mathbf{0}^{p\times 1} .$$

If $\mathbf{X}$ is of full rank p, that is

$$\mathbf{X} = \begin{pmatrix} x_{11} & x_{12} & \dots & x_{1p} \\ x_{21} & x_{22} & \dots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \dots & x_{np} \end{pmatrix}$$

where the rows

$$(x_{i1}, x_{i2}, \dots, x_{ip})$$

are linearly independent

$$\sum_{i=1}^{n} c_i(x_{i1}, x_{i2}, \dots, x_{ip}) = 0 \text{ if and only if } c_i = 0 \text{ for all } i = 1, 2, \dots, n,$$

then the solution is unique and is

$$\hat{\boldsymbol{\beta}} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{Y}$$

although this is not the best way to calculate it. Following the discussion in chapter 11, for the full rank case, we can use the $\mathbf{QR}$ decomposition

$$\mathbf{X} = \mathbf{QR}$$

where $\mathbf{Q}^{n\times n}$ is orthogonal and

$$R^{n\times p} = \begin{pmatrix} r_{11} & r_{12} & \dots & r_{1p} \\ 0 & r_{22} & \dots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & r_{pp} \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix} = \begin{pmatrix} \mathbf{R}_{11}^{p\times p} \\ \mathbf{0}^{(n-p)\times p} \end{pmatrix}$$

with $r_{ii} > 0$. Then

$$\hat{\boldsymbol{\beta}} = \mathbf{R}_{11}^{-1}\mathbf{Q}_1^T\mathbf{Y}$$

is obtained by solving backward the triangular linear equation

$$\mathbf{R}_{11}\boldsymbol{\beta} = \mathbf{Q}_1^T\mathbf{Y}$$

where the partition

$$\mathbf{Q}^T = \begin{pmatrix} \mathbf{Q}_1^T \\ \mathbf{Q}_2^T \end{pmatrix}$$

and $\mathbf{Q_1^T}$ and $\mathbf{Q_2^T}$ are of dimension $p \times n$ and $(n-p) \times n$ respectively.

The **QR** decomposition can be obtained by Householder transformations as illustrated in program **Regress.cpp**..

Since $\hat{\boldsymbol{\beta}}$ is a function of the complete sufficient statistic $\mathbf{X^TY}$ and $\mathbf{Y^TY}$ and has the normal distribution

$$\hat{\boldsymbol{\beta}} : \mathcal{N}_p(\boldsymbol{\beta}, \sigma^2(R_{11}^T R_{11})^{-1}) = \mathcal{N}_p(\boldsymbol{\beta}, \sigma^2(\mathbf{X^TX})^{-1})$$

it is unbiased and is the UMVU estimator of $\boldsymbol{\beta}$. It is also the m.l.e. estimator of $\boldsymbol{\beta}$.

14.2 The UMVU Estimator for σ^2

From chapter 11, we have the U.M.V.U. estimator for σ^2 is

$$\mathcal{S}^2(\hat{\boldsymbol{\beta}}) = \frac{\mathbf{W^TW}}{(n-p)}$$

where $\mathbf{W} = Q_2^T\mathbf{Y}$ has the normal distribution $\mathcal{N}_{(n-p)}(0, \sigma^2\mathbf{I}_{(n-p)})$ so that $\mathcal{S}^2(\hat{\boldsymbol{\beta}})$ is distributed as $(\sigma^2/(n-p))\chi^2_{(n-p)}(0)$.

We note that $\hat{\boldsymbol{\beta}}$ is a function of $\mathbf{V} = \mathbf{Q}_1^T\mathbf{Y}$ and $\mathcal{S}^2(\hat{\boldsymbol{\beta}})$ is a function of $\mathbf{W} = \mathbf{Q}_2^T\mathbf{Y}$ so that $\hat{\boldsymbol{\beta}}$ and $\mathcal{S}^2(\hat{\boldsymbol{\beta}})$ are statistically independent since $\mathbf{V}, \mathbf{W}$ have normal distributions and

$$Cov(\mathbf{V}, \mathbf{W}) = \mathbf{0}$$

because $\mathbf{Q}_1^T\mathbf{Q}_2 = \mathbf{0}$ from the orthogonality of $\mathbf{Q}$.

14.3 The Linear Hypothesis

For the full rank case $(r = p)$ we next consider the hypothesis

$$H: \ \mathbf{A}_0\boldsymbol{\beta} = \mathbf{c}_0 \text{ versus the alternative } A: \ \mathbf{A}_0\boldsymbol{\beta} \neq \mathbf{c}_0$$

where $\mathbf{A}_0^{m\times p}$, of full rank m $(m < p < n)$, and for

$$\mathbf{A}_0 = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1p} \\ a_{21} & a_{22} & \dots & a_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mp} \end{pmatrix}$$

we have the rows of $\mathbf{A}_0$ are linear combinations of the rows of $\mathbf{X}$, that is

$$(a_{i1}, a_{i2}, \dots, a_{ip}) = \sum_{j=1}^{n} d_{ij}(x_{i1}, x_{i2}, \dots, x_{ip})$$

for some constants d_{ij}, $i = 1, 2, \dots, m$, not all zero. $\mathbf{A}_0$ and $\mathbf{c}_0^{m\times 1}$ are both known.

Consider the problem of finding the $\boldsymbol{\beta} = \hat{\boldsymbol{\beta}}_0$ that minimizes

$$\mathcal{S}^2(\boldsymbol{\beta}) = \sum_{i=1}^{n}(Y_i - \sum_{j=1}^{p} x_{ij}\beta_j)^2$$

subject to $\mathbf{A}_0\boldsymbol{\beta} = \mathbf{c}_0$. We can differentiate the Lagrange Multiplier

$$\mathcal{L}(\boldsymbol{\beta}) = (\mathbf{Y} - \mathbf{X}\boldsymbol{\beta})^T(\mathbf{Y} - \mathbf{X}\boldsymbol{\beta}) - 2\boldsymbol{\lambda}^T(\mathbf{A}_0\boldsymbol{\beta} - \mathbf{c}_0)$$

and solve the equation set to zero to obtain the constrained minimizing value

$$\hat{\boldsymbol{\beta}}_0 = \hat{\boldsymbol{\beta}} - (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T(\mathbf{A}_0(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T)^{-1}(\mathbf{A}_0\hat{\boldsymbol{\beta}} - \mathbf{c}_0)\ .$$

Using $\mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}^T\mathbf{Y}$ to simplify, we obtain the value

$$\mathcal{S}^2(\hat{\boldsymbol{\beta}}_0) = \mathcal{S}^2(\hat{\boldsymbol{\beta}}) + \mathcal{S}_H^2$$

where

$$\mathcal{S}_H^2 = (\mathbf{A}_0\hat{\boldsymbol{\beta}} - \mathbf{c}_0)^T(\mathbf{A}_0(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T)^{-1}(\mathbf{A}_0\hat{\boldsymbol{\beta}} - \mathbf{c}_0)\ . \tag{14.1}$$

The generalized likelihood ratio test then can be reduced to rejecting the hypothesis H in favor of the alternative A if

$$\mathcal{F} = \frac{\mathcal{S}_H^2/m}{\mathcal{S}^2(\hat{\beta})/(n-p)} > F_{\alpha,m,(n-p)}$$

where $F_{\alpha,m,(n-p)}$ is the upper α probability point of the central F distribution with degrees of freedom $(m, n-p)$. We note that $\mathcal{S}_\omega^2$ and $\mathcal{S}^2(\hat{\beta})$ are statistically independent since they are functions of $\mathbf{V}$ and $\mathbf{W}$ respectively.

The distribution of $\mathcal{F}$ under the alternative is that of a noncentral F with noncentrality parameter

$$\delta^2 = \frac{(\mathbf{A}_0\boldsymbol{\beta} - \mathbf{c}_0)^T(\mathbf{A}_0(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T)^{-1}(\mathbf{A}_0\boldsymbol{\beta} - \mathbf{c}_0)}{\sigma^2}$$

and degrees of freedom $(m, n-p)$. Equivalently,

$$U = \frac{\mathcal{S}_\omega^2}{\mathcal{S}_\omega^2 + \mathcal{S}^2(\hat{\boldsymbol{\beta}})}$$

has the noncentral beta$(m/2, (n-p)/2, \delta^2)$ distribution with the same noncentrality parameter δ^2.

As an example, consider the two-way layout with equal numbers per cell:

$$Y_{jkl} = \mu_{jk} + \varepsilon_{jkl} \text{ for } j = 1, 2, \ldots, J, \quad k = 1, 2, \ldots, K, \quad l = 1, 2, \ldots, L \tag{14.2}$$

where ε_{jkl} are independent $\mathcal{N}(0, \sigma^2)$. Here

$$\boldsymbol{\beta}^T = (\mu_{11}, \mu_{12} \ldots, \mu_{1K}, \mu_{21} \ldots, \mu_{2K}, \ldots, \mu_{J1}, \ldots, \mu_{JK}),$$

$n = JKL$, $p = JK$. and $\mathbf{X}$ is the Kronecker product

$$\mathbf{X}^{JKL\times JK} = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 1 & 0 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix} = \mathbf{I}_{JK} \otimes \mathbf{1}_L$$

where $\mathbf{I}_{JK}$ is the $JK \times JK$ identity matrix and $\mathbf{1}_L$ is the column vector of 1's of length L. Note the Kronecker product $A \otimes B$ is

$$A^{m\times n} \otimes B^{r\times s} = C^{mr\times ns} = \begin{pmatrix} a_{11}B & a_{12}B & \dots & a_{1n}B \\ a_{21}B & a_{22}B & \dots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mn}B \end{pmatrix}.$$

If

$$A^{3\times 2} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} \text{ and } B^{2\times 2} = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

then

$$A \otimes B = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} & a_{13}b_{11} & a_{13}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{22}b_{12} & a_{13}b_{21} & a_{13}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} & a_{23}b_{11} & a_{23}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} & a_{23}b_{21} & a_{23}b_{22} \end{pmatrix}^{6\times 4}.$$

For the hypothesis for the row effects

$$H_1 : \mu_{j\cdot} - \mu_{\cdot\cdot} = 0 \text{ versus } A_1 : \mu_{j\cdot} - \mu_{\cdot\cdot} \neq 0 \text{ for } j = 1, 2, \dots, J-1$$

(note under H_1 we also have $\mu_{J\cdot} - \mu_{\cdot\cdot} = 0$ since $\sum_{j=1}^{J}(\mu_{j\cdot} - \mu_{\cdot\cdot} = 0)$ where

$$\mu_{j\cdot} = \sum_{k=1}^{K} \mu_{jk}/K, \quad \mu_{\cdot\cdot} = \sum_{j=1}^{J}\sum_{k=1}^{K} \mu_{jk}/(JK)$$

we have $\mathbf{A}_0^{(J-1)\times JK} =$

$$\begin{pmatrix} \frac{1}{K} - \frac{1}{JK} & \dots & \frac{1}{K} - \frac{1}{JK} & -\frac{1}{JK} & \dots & -\frac{1}{JK} & \dots & -\frac{1}{JK} & \dots & -\frac{1}{JK} \\ -\frac{1}{JK} & \dots & -\frac{1}{JK} & \frac{1}{K} - \frac{1}{JK} & \dots & \frac{1}{K} - \frac{1}{JK} & \dots & -\frac{1}{JK} & \dots & -\frac{1}{JK} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \ddots & \vdots \\ -\frac{1}{JK} & \dots & -\frac{1}{JK} & -\frac{1}{JK} & \dots & -\frac{1}{JK} & \ddots & -\frac{1}{JK} & \dots & -\frac{1}{JK} \end{pmatrix}$$

$$= \frac{1}{K} \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix}^{(J-1)\times J} \otimes \mathbf{1}_K^T - \frac{1}{JK}\mathbf{1}_{(J-1)}\mathbf{1}_{JK}^T$$

and $\mathbf{c}_0^{(J-1)\times 1} = \mathbf{0}$. Then we obtain

$$(\mathbf{X}^T\mathbf{X})^{-1} = \frac{1}{L}\mathbf{I}_{JK}$$

$$(\mathbf{A}_0((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T) = \left(\frac{1}{KL}\mathbf{I}_{J-1} - \frac{1}{J}\mathbf{1}_{(J-1)}\mathbf{1}_{(J-1)}^T\right)$$

$$(\mathbf{A}_0((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T)^{-1} = KL\left(\mathbf{I}_{(J-1)} + \mathbf{1}_{(J-1)}\mathbf{1}_{(J-1)}^T\right) \ .$$

$$\mathcal{S}_{H_1}^2 = (\mathbf{A}_0\hat{\boldsymbol{\beta}} - \mathbf{c}_0)^T(\mathbf{A}_0(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T)^{-1}(\mathbf{A}_0\hat{\boldsymbol{\beta}} - \mathbf{c}_0) = KL\sum_{j=1}^{J}(Y_{j\cdot\cdot} - Y_{\cdots})^2 \tag{14.3}$$

with degrees of freedom $\nu_1 = (J-1)$. The $\mathcal{F}$ statistic is then

$$\mathcal{F} = \frac{\mathcal{S}_{H_1}^2/(J-1)}{\mathcal{S}_e^2/(JK(L-1))} = \frac{KL\sum_{j=1}^{J}(Y_{j\cdot\cdot} - Y_{\cdots})^2/(J-1)}{\sum_{j=1}^{J}\sum_{k=1}^{K}\sum_{l=1}^{L}(Y_{jkl} - Y_{jk\cdot})^2/(JK(L-1))} \ .$$

Similarly for the hypotheses for the column effects and interactions

$$H_2: \ \mu_{\cdot k} - \mu_{\cdot\cdot} = 0 \text{ for } k = 1, 2, \ldots K-1$$

$$H_{12}: \ \mu_{jk} - \mu_{j\cdot} - \mu_{\cdot k} + \mu_{\cdot\cdot} = 0 \text{ for } j = 1, 2, \ldots J-1, \ k = 1, 2, \ldots, K-1$$

we have the sums of squares $\mathcal{S}^2$ and degrees of freedom ν are respectively

$$\mathcal{S}_{H_2}^2 = JL\sum_{k=1}^{K}(Y_{\cdot k\cdot} - Y_{\cdots})^2, \quad \nu_2 = (K-1)$$

$$\mathcal{S}_{H_{12}}^2 = L\sum_{j=1}^{J}\sum_{k=1}^{K}(Y_{jk\cdot} - Y_{j\cdot\cdot} - Y_{\cdot k\cdot} + Y_{\cdots})^2, \quad \nu_{12} = (J-1)(K-1)$$

The denominator sum of squares and degrees of freedom are

$$\mathcal{S}_e^2 = \sum_{j=1}^{J}\sum_{k=1}^{K}\sum_{l=1}^{L}(Y_{jkl} - Y_{jk\cdot})^2, \quad \nu_e = JK(L-1) \ . \tag{14.4}$$

The computations are often presented in an analysis of variance table

Source	SS	d.f.	MS	$\mathcal{F}$	P-value
Rows	$\mathcal{S}^2_{H_1}$	ν_1	MS_1	MS_1/MS_e	$P(F_{\nu_1,\nu_e} > \frac{MS_1}{MS_e})$
Columns	$\mathcal{S}^2_{H_2}$	ν_2	MS_2	MS_2/MS_e	$P(F_{\nu_2,\nu_e} > \frac{MS_2}{MS_e})$
Interactions	$\mathcal{S}^2_{H_{12}}$	ν_{12}	MS_{12}	MS_{12}/MS_e	$P(F_{\nu_{12},\nu_e} > \frac{MS_{12}}{MS_e})$
Error	$\mathcal{S}^2_e$	ν_e	MS_e		
Total	$\mathcal{S}^2_T$	ν_T	MS_T		

Here SS stands for the sum of squares, $d.f.$ for the degrees of freedom, and MS for the mean squares ($SS/d.f.$). The total sum of squares and degrees of freedom are

$$\mathcal{S}^2_T = \sum_{j=1}^{J}\sum_{k=1}^{K}\sum_{l=1}^{L}(Y_{jkl} - Y_{...})^2, \quad \nu_T = JKL - 1$$

and, for this balanced case, are calculated as a check sum of all the SS and degrees of freedom.

For specific linear models, more direct methods are often used to more easily calculate the sums of squares.

14.4 Latin Squares

Consider the latin square design with M^2 observations

$$Y_{i,j,k(ij)} = \mu + \alpha_i + \beta_j + \gamma_{k(ij} + \varepsilon_{i,j,k(ij)}$$

where $\varepsilon_{i,j,k}$ are independent $\mathcal{N}(0,\sigma^2)$, $\alpha_. = \beta_. = \gamma_. = 0$ with indices $i = 1,2,\ldots,M$, $j = 1,2,\ldots,M$ and $k = k(ij)$ determined by a Latin square design from an array of $k(ij)$ values. In the ith row $k(ij)$ has all the values $1,2,\ldots,M$ and in the jth column $k(ij)$ also has all the values $1,2,\ldots,M$. For example, with $M = 5$ table 14.1 is a 5×5 latin square:

Hypotheses of interest are $H_A:\ \alpha_i = 0$ for all $i = 1,2,\ldots,M$, $H_B:\ \beta_j = 0$ for all $j = 1,2,\ldots,M$ and $H_C:\ \gamma_k = 0$ for all $k = 1,2,\ldots,M$. After minimizing the sums of squares directly, we get the ANOVA table

Table 14.1: A Latin Square 5×5.

k	j				
i	1	2	3	4	5
	2	3	4	5	1
	3	4	5	1	2
	4	5	1	2	2
	5	1	2	3	4

Source	SS	D.F.	MS	F
A	$S_A^2 = M\sum_{i=1}^M (Y_{i\cdot\cdot} - Y_{\cdots})^2$	$M-1$	$MS_A = \frac{S_A^2}{M-1}$	$\frac{MS_A}{MS_e}$
B	$S_B^2 = M\sum_{j=1}^M (Y_{\cdot j\cdot} - Y_{\cdots})^2$	$M-1$	$MS_B = \frac{S_B^2}{M-1}$	$\frac{MS_B}{MS_e}$
C	$S_C^2 = M\sum_{k=1}^M (Y_{\cdot\cdot k} - Y_{\cdots})^2$	$M-1$	$MS_C = \frac{S_C^2}{M-1}$	$\frac{MS_C}{MS_e}$
Error	S_e^2	DF_e	$MS_e = \frac{S_e^2}{DF_e}$	
Total	$S_T^2 = \sum_{i=1}^M \sum_{j=1}^M (Y_{i,j,k(ij)} - Y_{\cdots})^2$	M^2-1	$MS_T = \frac{S_T^2}{M^2-1}$	

where $DF_e = M^2 - 3M + 2$, $\quad Y_{\cdots} = \sum_{i=1}^M \sum_{j=1}^M Y_{i,j,k(ij)}/M^2$,

$$S_e^2 = \sum_{i=1}^m \sum_{j=1}^M (Y_{i,j,k(ij)} - Y_{i\cdot\cdot} - Y_{\cdot j\cdot} - Y_{\cdot\cdot k(ij)} + 2Y_{\cdots})^2 \ ,$$

and

$$Y_{\cdot\cdot k} = \frac{1}{M} \sum_{(i,j)\in D_k} Y_{i,j,k(ij)} \ , \quad D_k = \{(i,j) : k(ij) = k\} \ .$$

14.5 Unbalanced Multifactor ANOVA

We consider a contrast algorithm following Scheffé (1959) [1] and extended by Jorn and Klotz (1989)[2] [3]

[1] Scheffé, H.(959) *The Analysis of Variance*, John Wiley and Sons, New York section 3.5

[2] H. Jorn and J. Klotz (1989) The contrast algorithm for unbalanced multifactor analysis of variance. *Journal of the American Statistical Association* **84**, pages 318-324.

[3] H. Jorn *An Algorithm for Unbalanced Multifactor ANOVA Models with Contrasts.* 1986 PhD thesis, University of Wisconsin, Department of Statistics.

Consider the multifactor analysis of variance model with treatment factors $1, 2, \ldots, p$, each of which has levels $L_1, L_2, \ldots, L_p$. Let $\mathbf{i} = (i_1, i_2, \ldots i_p)$ where $i_r \in \{1, 2, \ldots, L_r\}$ be a vector of integers that represent a particular combination of treatment levels or *cell*. Assume there are $n(\mathbf{i}) > 0$ observations there and write the j-th observation as

$$Y_j(\mathbf{i}) = \mu(\mathbf{i}) + \varepsilon(\mathbf{i}) \text{ for } j = 1, 2, \ldots, n(\mathbf{i}) \ .$$

The parameter $\mu(\mathbf{i})$ is the cell expectation and the random variable $\varepsilon(\mathbf{i})$ is the error term assumed to be independent $\mathcal{N}(0, \sigma^2)$ for all $\mathbf{i}$ and j.

We define overall effect, main effects, and higher order interactions as weighted combinations of cell expectations. For the r-th factor, define weight $w_r(i_r)$ for level i_r, where $\sum_{i_r=1}^{L_r} w_r(i_r) = 1$. Equal weights $w_r(i_r) = 1/L_r$ are most commonly used but unequal weights can emphasize certain levels of a factor.

Define constant, main, and higher order interactions by

$$m = \mu(\cdot, \cdot, \ldots, \cdot) = \sum_{i_1} \sum_{i_2} \ldots \sum_{i_p} w_1(i_1) w_2(i_2) \ldots w_p(i_p) \mu(i_1, i_2, \ldots, i_p),$$

$$m_r(i_r) = \mu(\cdot, \ldots, \cdot, i_r, \cdot, \ldots, \cdot) - m$$

$$m_{rs}(i_r, i_s) = \mu(\cdot, \ldots, \cdot, i_r, \cdot, \ldots, i_s, \cdot, \ldots, \cdot) - m - m_r(i_r) - m_s(i_s)$$

$\ldots$

$$m_{12\ldots p}(i_1, i_2, \ldots, i_p) = \mu(i_i, i_2, \ldots, i_p) - m - \sum_{r=1}^{p} m_r(i_r) - \sum_{i \le r} \sum_{< s \le p} m_{rs}(i_r, i_s) - \ldots - \text{etc.}$$

where the $(\cdot)$ notation in the r-th position indicates weighted averaging on the r-th factor. The main effects and interactions satisfy side conditions

$$m_r(\cdot) = \sum_{i_r=1}^{L_r} w_r(i_r) m_r(i_r) = 0, \quad m_{rs}(i_r, \cdot) = m_r(\cdot, i_s) = 0$$

$$m_{rst}(i_r, i_s, \cdot) = m_{rst}(i_r, \cdot, i_t) = m_{rst}(\cdot, i_s, i_t) = 0, \text{ etc.}$$

This provides a reparameterization with

$$\mu(\mathbf{i}) = m + \sum_{r=1}^{p} m_r(i_r) + \sum_{i \le r} \sum_{< s \le p} m_{rs}(i_r, i_s) + \ldots + m_{12\ldots p}(i_1, i_2, \ldots, i_p) \ .$$

Hypotheses of interest are

$$H_{r_1 r_2 \ldots r_k} : \; m_{r_1 r_2 \ldots r_k}(i_{r_1}, i_{r_2}, \ldots, i_{r_k}) = 0 \text{ for all } i_{r_1}, i_{r_2}, \ldots, i_{r_k} \; . \tag{14.5}$$

To calculate the numerator sums of squares for these hypotheses, many algorithms solve linear equations $\mathbf{X}^T\mathbf{X}\beta = \mathbf{X}^T\mathbf{Y}$ to minimize the sum of squares and then subtract an error sum of squares. While this approach is quite general for many different models, it lacks efficiency in our specific case and can lead to floating point inaccuracy when subtracting the error sum of squares if there are common leading digits. We propose a more efficient algorithm based on Scheffé's method of multiple comparisons which does not require the error sum of squares subtraction.

Hypotheses (14.5) hold if and only if all linear combinations of the parameters are zero. In particular, H_r holds if and only if linear combinations

$$\psi_r = \sum_{i_r=1}^{L_r} c(i_r) m_r(i_r) = 0$$

for all $\{c(i_r) : \; i_r = 1, 2, \ldots L_r\}$. The hypotheses H_{rs} hold if and only if

$$\psi_{rs} = \sum_{i_r=1}^{L_r} \sum_{i_s=1}^{L_s} c(i_r, i_s) m_{rs}(i_r, i_s) = 0$$

for all $\{c(i_r, i_s) : \; i_r = 1, 2, \ldots L_r, i_s = 1, 2, \ldots, L_s\}$ with similar zero linear combinations for higher order interactions.

Scheffé (1959), section 3.5, proves that the numerator sum of squares corresponding to a general linear hypothesis is equivalent to the square of the maximal linear combination estimate among those that satisfy a variance constraint:

$$S_H^2 = \hat{\psi}_{max}^2, \text{ where } \mathrm{Var}(\hat{\psi}_{max}^2) = \sigma^2 \; .$$

To describe the calculation of $\hat{\psi}_{max}^2$, consider the k-th order interaction where we simplify notation by choosing the first k factors. Calculations for other subsets are similar. For $H_{12\ldots k}$ defined in (14.5) consider

$$\psi_{12\ldots k} = \sum_{i_1=1}^{L_1} \sum_{i_2=1}^{L_2} \cdots \sum_{i_k=1}^{L_K} c(i_1, i_2, \ldots, i_k) m_{12\ldots k}(i_1, i_2, \ldots, i_k) \; .$$

Since $m_{12\ldots k}(i_1, i_2, \ldots, i_k)$ is a linear combination of cell means, we can write $\psi_{12\ldots k}$ as

$$\psi_{12\ldots k} = \sum_{i_1=1}^{L_1} \sum_{i_2=1}^{L_2} \cdots \sum_{i_k=1}^{L_K} d(i_1, i_2, \ldots, i_k)\mu(i_1, i_2, \ldots, i_k) \tag{14.6}$$

which we call a *contrast*. The coefficients $d(i_1, i_2, \ldots, i_k) =$

$$c(i_1, i_2, \ldots, i_k) - w_1(i_1)c(+, i_2, \ldots, i_k) - \ldots - w_k(i_k)c(i_1, i_2, \ldots, i_{k-1}, +)$$

$$+w_1(i_1)w_2(i_2)c(+, +, i_3, \ldots, i_k) + w_1(i_1)w_3(i_3)c(+, i_2, +, i_4, \ldots, i_k) + \ldots$$

$$+w_{k-1}(i_{k-1})w_k(i_k)c(i_1, i_2, \ldots, i_{k-2}, +, +) + \ldots$$

p

$$+(-1)^k w_1(i_1)w_2(i_2)\ldots w_k(i_k)c(+, +, \ldots, +) \tag{14.7}$$

where $c(+, i_2, \ldots, i_k) = \sum_{i_1=1}^{L_i} c(i_1, i_2, \ldots, i_k)$. In matrix notation,

$$\mathbf{d} = ((\mathbf{I}_{L_1} - \mathbf{w}_1\mathbf{1}_{L_1}^T) \otimes (\mathbf{I}_{L_2} - \mathbf{w}_2\mathbf{1}_{L_2}^T) \otimes \ldots \otimes (\mathbf{I}_{L_k} - \mathbf{w}_k\mathbf{1}_{L_k}^T))\mathbf{c}$$

where $\mathbf{w}_r$ is the column vector of weights for factor r and $\mathbf{c}$ and $\mathbf{d}$ are column vectors in lexical order of their arguments $(i_1, i_2, \ldots, i_k)$.

The rank of $(\mathbf{I}_{L_r} - \mathbf{w}_r\mathbf{1}_{L_r}^T)$ is $(L_r - 1)$ so the linear space of vectors $\mathbf{d}$ has rank $\prod_{r-1}^k (L_r - 1)$ using the rank of a Kronecker product is the product of the ranks.

It follows from (14.7) for $s = 1, 2, \ldots, k$ we have

$$\sum_{i_s=1}^{L_s} d(i_1, i_2, \ldots, i_k) = 0 \text{ for all } i_r \text{ with } r \neq s\ . \tag{14.8}$$

Although there are a total of $\sum_{s=1}^k \{\prod_{r=1}^k L_r/L_s\}$ equations in (14.8), only a total of

$$\nu = (\prod_{r=1}^k L_r) - (\prod_{r=1}^k (L_r - 1)) \tag{14.9}$$

constraints can be independent because of the rank of the $\mathbf{d}$ space. We replace equations (14.8) by an equivalent independent subset of equations

$$\sum_{i_1=1}^{L_1} d(i_1, i_2, \ldots, i_k) = 0 \text{ for all } i_t = 1, 2, \ldots, L_t, \text{ for } t > 1,$$

$$\sum_{i_s=1}^{L_s} d(i_1, i_2, \ldots, i_k) = 0 \text{ for all } i_r = 1, 2, \ldots, L_r - 1, \text{ and}$$

$$\text{for all } i_t = 1, 2, \ldots, L_t \text{ where } 1 \le r < s < t \le k,$$

$$\sum_{i_k=1}^{L_k} d(i_1, i_2, \ldots, i_k) = 0 \text{ for all } i_r = 1, 2, \ldots, L_r - 1 \text{ where } r < k\ . \quad (14.10)$$

The total number of constraints in equations (14.10) is

$$\nu = \prod_{t=2}^{k} L_t + \sum_{s=2}^{k-1}(\prod_{r=1}^{s-1}(L_r - 1)(\prod_{t=s+1}^{k} L_t) + \prod_{r=1}^{k-1}(L_t - 1)\ . \quad (14.11)$$

The equality of (14.9) and (14.11) can be shown by induction on k.

To estimate $\psi_{12\ldots k}$ replace $\mu(\mathbf{i})$ by the cell average $Y_{\cdot}(\mathbf{i})$ to obtain

$$\hat{\psi}_{12\ldots k} = \sum_{i_1=1}^{L_1}\sum_{i_2=1}^{L_2}\cdots\sum_{i_k=1}^{L_k} d(i_1, i_2, \ldots, i_k) Y_{\cdot}(i_1, i_2, \ldots, i_k, \cdot, \ldots, \cdot)\ . \quad (14.12)$$

Define $V_{12\ldots k}$ by

$$\mathrm{Var}(Y_{\cdot}(i_1, i_2, \ldots, i_k, \cdot, \ldots, \cdot)) = \sigma^2 / V_{12\ldots k}(i_1, 1_2, \ldots, i_k)$$

or

$$V_{12\ldots k}(i_1, 1_2, \ldots, i_k) = (\sum_{i_{k+1}=1}^{L_{k+1}} \cdots \sum_{i_p=1}^{L_p} w_{k+1}^2(i_{k+1}) \cdots w_p^2(i_p)/n(i_1, i_2, \ldots, i_p))^{-1}$$

with $V_{12\ldots k}(\mathbf{i}) = n(\mathbf{i})$. Then

$$\mathrm{Var}(\hat{\psi}_{12\ldots k}) = \sigma^2 \sum_{i_1=1}^{L_1}\sum_{i_2=1}^{L_2}\cdots\sum_{i_k=1}^{L_k} d^2(i_1, i_2, \ldots, i_k)/V_{12\ldots k}(i_1, i_2, \ldots, i_k) \quad (14.13)$$

To obtain $S_{12\ldots k}^2 = \hat{\psi}_{max}^2$ we calculate $\hat{\psi}_{max}$ by maximizing (14.12) with respect to choice of $\mathbf{d}$ subject to constraints (14.10) and

$$\sum_{i_1=1}^{L_1}\sum_{i_2=1}^{L_2}\cdots\sum_{i_k=1}^{L_k} d^2(i_1, i_2, \ldots, i_k)/V_{12\ldots k}(i_1, i_2, \ldots, i_k) = 1 \quad (14.14)$$

from $\mathrm{Var}(\hat{\psi}_{max}) = \sigma^2$ and (14.13). The Lagrange multiplier equation for this constrained maximization problem is:

$$\mathcal{L} = \sum_{i_1=1}^{L_1}\sum_{i_2=1}^{L_2}\cdots\sum_{i_k=1}^{L_k} d(i_1, i_2, \ldots, i_k) Y_{\cdot}(i_1, i_2, \ldots, i_k, \cdot, \ldots, \cdot)$$

$$-\frac{\lambda_0}{2}\{\sum_{i_1=1}^{L_1}\sum_{i_2=1}^{L_2}\cdots\sum_{i_k=1}^{L_k} d^2(i_1, i_2, \ldots, i_k)/V_{12\ldots k}(i_1, i_2, \ldots, i_k) - 1\}$$

$$-\sum_{i_2=1}^{L_2}\cdots\sum_{i_k=1}^{L_k}\lambda_1(i_2, \ldots, i_k)\sum_{i_1=1}^{L_1} d(i_1, \ldots, i_k)$$

$$-\sum_{i_1=1}^{L_1}\sum_{i_3=1}^{L_3}\cdots\sum_{i_k=1}^{L_k}\lambda_2(i_1, i_3, \ldots, i_k)\sum_{i_2=1}^{L_2} d(i_1, \ldots, i_k) - \ldots$$

$$-\sum_{i_1=1}^{L_1-1}\cdots\sum_{i_{k-1}=1}^{L_{k-1}-1}\lambda_k(i_1, \ldots, i_{k-1})\sum_{i_k=1}^{L_k} d(i_1, \ldots, i_k)\ . \tag{14.15}$$

Note for values of $d(i_1, \ldots, i_k)$ that maximize (14.12) subject to (14.14) and (14.10), the resulting value of $\mathcal{L}$ gives $\hat{\psi}_{max}$ since all but the first term in (14.15) vanish. If we use the convention that $\lambda_s(i_1, \ldots, i_{s-1}, i_{s+1}, \ldots, i_k) = 0$ for $i_r = L_r$ with $r < s$, since these terms are absent in (14.15), and drop the arguments $(i_1, \ldots, i_k)$ to save space, we can write

$$\mathcal{L} = \sum_{i_1}\cdots\sum_{i_k} d(Y_{\cdot} - \lambda_1 - \lambda_2 - \cdots - \lambda_k) - (\lambda_0/2)(\sum_{i_1}\cdots\sum_{i_k} d^2/V_{12\ldots k} - 1)\ .$$

Differentiating $\mathcal{L}$ with respect to $d(i_1, \ldots, i_k)$ and equating to zero gives

$$d = (Y_{\cdot} - \lambda_1 - \lambda_2 - \cdots - \lambda_k)V_{12\ldots k}/\lambda_0\ .$$

Substituting d into (14.14) gives

$$\lambda_0^2 = \sum_{i_1}\cdots\sum_{i_k} V_{12\ldots k}(Y_{\cdot} - \lambda_1 - \lambda_2 - \cdots - \lambda_k)^2\ .$$

Finally, replacing d and λ_0 in $\mathcal{L}$ gives

$$\hat{\psi}_{max} = \mathcal{L} = \sum_{i_1}\cdots\sum_{i_k} V_{12\ldots k}(Y_{\cdot} - \lambda_1 - \lambda_2 - \cdots - \lambda_k)^2/\lambda_0$$

$$= (\sum_{i_1} \cdots \sum_{i_k} V_{12\ldots k}(Y_{\cdot} - \lambda_1 - \lambda_2 - \cdots - \lambda_k)^2)^{1/2}$$

for values $\lambda_1, \lambda_2, \ldots, \lambda_k$ that satisfy (14.10). The resulting interaction sum of squares is

$$S^2_{12\ldots k} = \hat{\psi}^2_{max} =$$

$$\sum_{i_1=1}^{L_1} \cdots \sum_{i_k=1}^{L_k} V_{12,\ldots k}(i_1, \ldots, i_k)\{Y_{\cdot}(i_1, \ldots, i_k, \cdot, \ldots, \cdot) - \lambda_1(i_2, \ldots i_k) - \cdots - \_k(i_1, \ldots, i_{k-1})\}^2 \tag{14.16}$$

where the Lagrange multipliers $\lambda_1, \lambda_2, \ldots, \lambda_k$ areobtained by substituting d values into (14.10) or equivalently by solving

$$\sum_{i_s=1}^{L_s} V_{12\ldots k}(i_1, \ldots, i_k)\{Y_{\cdot}(i_1, \ldots, i_k, \cdot, \ldots, \cdot)i - \lambda_1(i_2, \ldots i_k) - \cdots - \_k(i_1, \ldots, i_{k-1})\} = 0 \tag{14.17}$$

for $s = 1$ and $i_t = 1, 2, \ldots L_t$, $t > 1$ and $1 < s < k$, $i_r = 1, 2, \ldots, L_r - 1$, $i_t = 1, 2, \ldots, L_t$, $1 \le r < s < t \le k$, and $s = k$, $i_r = 1, 2, \ldots, L_r - 1$, $r < k$.

For $1 < s < k$ let $\boldsymbol{\lambda}_s$ be the column vector of Lagrange multipliers with elements $\lambda_s(\mathbf{i}^{(s)})$ written in lexical order of the arguments $\mathbf{i}^{(s)} = (i_1, \ldots, i_{s-1}, i_{s+1}, \ldots, i_k)$:

$$\boldsymbol{\lambda}_s^T = (\lambda_s(1, \ldots, 1, 1, \ldots, 1), \ldots, \lambda_s(L_1 - 1, \ldots, L_{s-1} - 1, L_{s+1}, \ldots, L_k)) \; .$$

Similarly let

$$\boldsymbol{\lambda}_1^T = (\lambda_1(1, \ldots, 1), \ldots, \lambda_1(L_2, \ldots, L_k))$$
$$\boldsymbol{\lambda}_k^T = (\lambda_1(1, \ldots, 1), \ldots, \lambda_1(L_1 - 1, \ldots, L_{k-1} - 1)) \; .$$

These equations can be written in symmetric matrix form

$$\mathbf{A}\boldsymbol{\lambda} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \cdots & \mathbf{A}_{1k} \\ & \mathbf{A}_{22} & \cdots & \mathbf{A}_{2k} \\ & & \ddots & \\ & & & \mathbf{A}_{kk} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda}_1 \\ \boldsymbol{\lambda}_2 \\ \vdots \\ \boldsymbol{\lambda}_k \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_k \end{pmatrix} = \mathbf{b} \tag{14.18}$$

where the block $\mathbf{A}_{ss'}$ is a $\nu_s \times \nu_{s'}$ submatrix with

$$\nu_s = (\prod_{r=1}^{s-1}(L_r - 1))(\prod_{t=s+1}^{k} L_t) \text{ for } 1 < s < k, \text{ and } \nu_1 = \prod_{t=2}^{k} L_t, \quad \nu_k = \prod_{r=1}^{k-1}(L_r - 1) \; .$$

Define the integer j to be the position corresponding to the argument $\mathbf{i}^{(s)}$ in the lexical ordering of $\boldsymbol{\lambda}_s$. Similarly, let j' correspond to $\mathbf{i}^{(s')}$. Then the (j, j') element of $A_{ss'}$ is defined as follows for diagonal blocks

$$A_{ss} = \text{diag}(V_{12\ldots(s-1)+(s+1)\ldots k}(\mathbf{i}^{(s)}) : \; j = 1, 2, \ldots, \nu_s; \; j \leftrightarrow \mathbf{i}^{(s)})$$

where

$$V_{12\ldots(s-1)+(s+1)\ldots k}(\mathbf{i}^{(s)}) = \sum_{i_s=1}^{L_s} V_{12\ldots k}(i_1, \ldots, i_s, \ldots, i_k)$$

For off diagonal blocks

$$A_{ss'} = (a_{jj'} : \; j = 1, 2, \ldots, \nu_s, j' = 1, 2, \ldots, \nu_{s'})$$

where we define $a_{jj'}$ as follows:

$$a_{jj'} = \begin{cases} V_{12\ldots k}(i_1, i_2, \ldots, i_k), & \text{if } \mathbf{i}^{(s)} \text{ and } \mathbf{i}^{(s')} \text{ are } \textit{compatible} \\ 0 & \text{otherwise} \end{cases} \tag{14.19}$$

where j corresponds to $\mathbf{i}^{(s)}$ and j' corresponds to $\mathbf{i}^{(s')}$. In the vector $(i_1, i_2, \ldots, i_k)$ for $V_{12\ldots k}$ in equation (14.19) the value for i_s is determined by its value in $\mathbf{i}^{(s')}$ and the value for $i_{s'}$ is determined by its value in $\mathbf{i}^{(s)}$. The remaing values of i_r are determined by the common values in $\mathbf{i}^{(s)}$ and $\mathbf{i}^{(s')}$.
For $(i_1, i_2, \ldots, i_k)$, $\mathbf{i}^{(s)} = (i_1, \ldots, i_{s-1}, i_{s+1}, \ldots, i_k)$, $\mathbf{i}^{(s')} = (i_1, \ldots, i_{s'-1}, i_{s'+1}, \ldots, i_k)$, we say $\mathbf{i}^{(s)}$ and $\mathbf{i}^{(s')}$ are *compatible* if the common $k-2$ coordinates of $(i_1, i_2, \ldots, i_k)$ excluding i_s and $i_{s'}$ have the same values in $\mathbf{i}^{(s)}$ as in $\mathbf{i}^{(s')}$.
For example, for $(i_1, i_2, i_3, i_4) = (1, 2, 4, 7)$ we have $\mathbf{i}^{(3)} = (1, 2, 7)$, and $\mathbf{i}^{(2)} = (1, 4, 7)$ are *compatible* since i_1 and i_4 are the same. The vectors $\mathbf{b}_s$ in (14.18) are defined by

$$b_{sj} = \sum_{i_s=1}^{L_s} V_{12\ldots k} Y_{\cdot}(i_1, \ldots, i_k, \cdot, \ldots, \cdot)$$

where again j corresponds to $\mathbf{i}^{(s)}$ in the lexical order of $\boldsymbol{\lambda}_s$.

For large systems, most of the vectors $\mathbf{i}^{(s)}$ and $\mathbf{i}^{(s')}$ are not compatible yielding a sparse matrix. Algorithms for sparse matrices are appropriate for such systems[4][5].

[4]Shu-Yen Ho (1990). Sparse Matrix Methods for Unbalanced Multifactor ANCOVA. PhD thesis, Department of Statistics, University of Wisconsin at Madison.

[5]Ho, S.H. and Klotz, J.H. (1992). Sparse matrix methods for unbalanced multifactor analysis of variance and covariance. *J. Statistical Computation and Simulation* **41** 55-72

Table 14.2: Unbalanced 3 factor data with $(L_1, L_2, L_3) = (4, 3, 2)$.

$i_1i_2i_3$	$n(\mathbf{i})$	$Y_j(\mathbf{i})$		$Y_.(\mathbf{i})$	$i_1i_2i_3$	$n(\mathbf{i})$	$Y_j(\mathbf{i})$		$Y_.(\mathbf{i})$
111	2	1.11	0.97	1.040	311	2	1.22	1.13	1.175
112	2	1.52	1.45	1.485	312	2	1.38	1.08	1.230
121	2	1.09	0.99	1.040	321	2	1.34	1.41	1.375
122	2	1.27	1.22	1.245	322	2	1.40	1.21	1.305
131	1	1.21		1.210	331	2	1.34	1.19	1.265
132	1	1.24		1.240	332	2	1.46	1.39	1.425
211	2	1.30	1.00	1.150	411	2	1.19	1.03	1.110
212	2	1.55	1.53	1.540	412	1	1.29		1.290
221	2	1.03	1.21	1.120	421	2	1.36	1.16	1.260
222	2	1.24	1.34	1.290	422	2	1.42	1.39	1.405
231	2	1.12	0.96	1.040	431	2	1.46	1.03	1.245
232	1	1.27		1.270	432	1	1.62		1.620

The error sum of squares and degrees of freedom are

$$S_e^2 = \sum_{i_1=1}^{L_1}\sum_{i_2=1}^{L_2}\cdots\sum_{i_p=1}^{L_p}\sum_{j=1}^{n[\mathbf{i}]}(Y_j(\mathbf{i}) - Y_.(\mathbf{i}))^2, \text{ and } \nu_e = N - L_1L_2\cdots L_p\ .$$

14.5.1 An Example

We illustrate the calculations using equal weights for the data of Snedecor[6] Table 12.10.1) as modified by Federer and Zelen[7] (1966 Table 1). See Table 14.2 above.

For example, in the main effect calculations for factor 1,

$$V_1(2) = \{\sum_{i_2=1}^{3}\sum_{i_3=1}^{2}\frac{w_2^2(i_2)w_3^2(i_3)}{n(2,i_2,i_3)}\}^{-1}$$

$$= \{\left(\frac{1}{3}\right)^2\left(\frac{1}{2}\right)^2\left(\frac{1}{2}+\frac{1}{2}+\frac{1}{2}+\frac{1}{2}+\frac{1}{2}+\frac{1}{2}+\frac{1}{1}\right)\}^{-1} = 10.2857,$$

[6]G.W. Snedecor (1956) *Statistical Methods.* Iowas State College Press, Ames, Iowa.

[7]W.T. Federer and M. Zelen (1966). Analysis of multifactor classifications with unequal numbers of observations. *Biometrics* **22**, 525-552.

Table 14.3: Main effect computation summary.

r		$i_r = 1$	2	3	4	$\mathbf{A}$	$\mathbf{b}$	λ	S_r^2
	W_1	0.25	0.25	0.25	0.25				
1	V_1	9	10.2857	12	9	40.2857	51.0377	1.2699	0.07665
	$Y_\cdot(i_1, \cdot, \cdot)$	1.2100	1.2350	1.2958	1.3219				
	W_2	0.3333	0.3333	0.3333					
2	V_2	14.2222	16	10.6667		40.8889	51.6469	1.2631	0.01001
	$Y_\cdot(\cdot, i_2, \cdot)$	1.2525	1.2550	1.2894					
	W_3	0.5	0.5						
3	V_3	22.1538	18			40.1538	50.4200	1.2557	0.3960
	$Y_\cdot(\cdot, \cdot, i_3)$	1.1692	1.3621						

$$Y_\cdot(2, \cdot, \cdot) = \sum_{i_2=1}^{3} \sum_{i_3=1}^{2} w_2(i_2) w_3(i_3) Y_\cdot(2, i_2, i_3) =$$

$$\left(\frac{1}{3}\right)\left(\frac{1}{2}\right)(1.150 + 1.540 + 1.120 + 1.290 + 1.040 + 1.270) = 1.2350,$$

$$A^{1\times 1} = \sum_{i_1=1}^{4} V_1(i_1) = 9 + 10.2857 + 12 + 9 = 40.2857,$$

$$\mathbf{b}^{1\times 1} = \sum_{i_1=1}^{4} V_1(i_1) Y_\cdot(i_1, \cdot, \cdot) =$$

$$9 \times 1.21 + 10.2857 \times 1.2350 + 12 \times 1.2958 + 9 \times 1.3217 = 51.0377,$$

$$\lambda_1 = A^{-1}\mathbf{b} = (40.2857)^{-1}(57.0377) = 1.2669$$

$$S_1^2 = \sum_{i_1=1}^{4} V_1(i_1)(Y_\cdot(i_1, \cdot, \cdot) - \lambda_1)^2 =$$

$$9(1.2100 - 1.2669)^2 + 10.2875(1.235 - 1.2669)^2 +$$

$$12(1.2958 - 1.2669)^2 + 9(1.3217 - 1.2669)^2 = 0.07665.$$

For the $(1, 2)$ interaction, table 3 summarizes the calculation of V_{12} and $Y_\cdot(i_1, i_2, \cdot)$.

Table 14.4: Values of V_{12} and $Y.(i_1, i_2, \cdot)$.

$i_1 i_2$	11	12	13	21	22	23	31	32	33	41	42	43
$V_{12}(i_1, i_2)$	4	4	2	4	4	2.6667	4	4	4	2.6667	4	2.6667
$Y.(i_1, i_2, \cdot)$	1.2625	1.1425	1.225	1.345	1.205	1.155	1.2025	1.34	1.345	1.2	1.3325	1.4325

For the $(1, 2)$ interaction, the equation $A\boldsymbol{\lambda} = \mathbf{b}$ from (14.18) is

$$\left(\begin{array}{ccc|ccc} 14\frac{2}{3} & 0 & 0 & 4 & 4 & 4 \\ 0 & 16 & 0 & 4 & 4 & 4 \\ 0 & 0 & 11\frac{1}{3} & 2 & 2\frac{2}{3} & 4 \\ \hline 4 & 4 & 2 & 10 & 0 & 0 \\ 4 & 4 & 2\frac{2}{3} & 0 & 10\frac{2}{3} & 0 \\ 4 & 4 & 4 & 0 & 0 & 12 \end{array}\right) \left(\begin{array}{c} \lambda_1(1) \\ \lambda_1(2) \\ \lambda_1(3) \\ \hline \lambda_2(1) \\ \lambda_2(2) \\ \lambda_2(3) \end{array}\right) = \left(\begin{array}{c} 18.44 \\ 20.08 \\ 14.73 \\ \hline 12.07 \\ 13.28 \\ 15.55 \end{array}\right)$$

For example, with $s = 2,\ j = 3,\ \mathbf{i}^{(s)} = (3)$ and

$$b_{23} = \sum_{i_2=1}^{3} V_{12}(3, i_2) Y.(3, i_2, \cdot) = 4 \times (1.2025 + 1.34 + 1.345) = 15.55\ .$$

The solution

$$\boldsymbol{\lambda}^T = (1.3175, 1.3102, 1.3485, -0.1138, -0.0775, -0.0296)\ .$$

Substituting into equation (14.16) with $\lambda_2(4) = 0$ gives

$$S_{12}^2 = \sum_{i_1=1}^{4} \sum_{i_2=1}^{3} V_{12}(i_1, i_2)(Y.(i_1, i_2, \cdot) - \lambda_1(i_2) - \lambda_2(i_1))^2 = 0.21232\ .$$

Similar calculations give $S_{13}^2 = 0.0897$ and $S_{23}^2 = 0.04557$.

For the single 3 factor interaction $(1, 2, 3)$, we have $V_{123}(\mathbf{i}) = n(\mathbf{i})$ and $Y.(\mathbf{i})$ given in table 1.

We have

$$A\boldsymbol{\lambda} = \mathbf{b} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ & A_{22} & A_{23} \\ & & A_{33} \end{pmatrix} \begin{pmatrix} \boldsymbol{\lambda}_1 \\ \boldsymbol{\lambda}_2 \\ \boldsymbol{\lambda}_3 \end{pmatrix} = \begin{pmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \mathbf{b}_3 \end{pmatrix} =$$

$$
\left(\begin{array}{cccccc|cccccc|cccccc}
8 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 2 & 0 & 2 & 0 & 2 & 0 & 2 & 0 \\
0 & 7 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 2 & 2 & 0 & 2 & 0 & 2 & 0 \\
0 & 0 & 8 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 2 & 0 & 0 & 2 & 0 & 2 & 0 & 2 \\
0 & 0 & 0 & 8 & 0 & 0 & 0 & 2 & 0 & 2 & 0 & 2 & 0 & 2 & 0 & 2 & 0 & 2 \\
0 & 0 & 0 & 0 & 7 & 0 & 1 & 0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 5 & 0 & 1 & 0 & 1 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
 & & & & & & 5 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 \\
 & & & & & & 0 & 5 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 \\
 & & & & & & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 \\
 & & & & & & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 \\
 & & & & & & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 2 & 2 \\
 & & & & & & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 2 & 2 \\
\hline
 & & & & & & & & & & & & 4 & 0 & 0 & 0 & 0 & 0 \\
 & & & & & & & & & & & & 0 & 4 & 0 & 0 & 0 & 0 \\
 & & & & & & & & & & & & 0 & 0 & 4 & 0 & 0 & 0 \\
 & & & & & & & & & & & & 0 & 0 & 0 & 4 & 0 & 0 \\
 & & & & & & & & & & & & 0 & 0 & 0 & 0 & 4 & 0 \\
 & & & & & & & & & & & & 0 & 0 & 0 & 0 & 0 & 4
\end{array}\right)
\left(\begin{array}{r}
1.0679 \\ 1.3743 \\ 1.2621 \\ 1.4029 \\ 1.2851 \\ 1.5399 \\ \hline -0.2055 \\ -0.1694 \\ -0.2654 \\ -0.2293 \\ 0.0254 \\ -0.1603 \\ \hline 0.2289 \\ -0.0025 \\ 0.3713 \\ 0.1198 \\ 0.0489 \\ 0.0750
\end{array}\right)
=
\left(\begin{array}{r}
8.95 \\ 9.80 \\ 9.59 \\ 10.49 \\ 8.31 \\ 6.98 \\ \hline 5.37 \\ 6.70 \\ 6.62 \\ 6.93 \\ 7.63 \\ 7.92 \\ \hline 5.05 \\ 4.57 \\ 5.38 \\ 4.82 \\ 4.81 \\ 5.36
\end{array}\right) .
$$

Substituting $\lambda_2(4, i_3) = 0$, $\lambda_3(4, i_2) = 0$, $\lambda_3(i_1, 3) = 0$ gives

$$
S^2_{123} = \sum_{i_1=1}^{4} \sum_{i_2=1}^{3} \sum_{i_3=1}^{2} n(\mathbf{i})(Y.(\mathbf{i}) - \lambda_1(i_2, i_3) - \lambda_2(i_1, i_3) - \lambda_3(i_1, i_2))^2 = 0.08362 .
$$

Table 4 gives the summary ANOVA table.

Table 4. ANOVA table for the data of table 1.

Source	SS	d.f.	MS	F	P-value
Main effects					
Factor 1	0.07665	3	0.02555	1.5830	0.2264
Factor 2	0.01001	2	0.00501	0.3102	0.7370
Factor 3	0.36960	1	0.36960	22.9010	0.0001
2-way interactions					
Factor 1×2	0.21232	6	0.03539	2.1926	0.0893
Factor 1×3	0.08097	3	0.02699	1.6723	0.2066
Factor 2×3	0.04557	2	0.02279	1.4118	0.2681
3-way interaction					
Factor 1×2×3	0.08362	6	0.01394	0.8635	0.5389
Error	0.30665	19	0.01614		
Total	1.2429	42			

The C++ program **multiway.cpp** in **Appendix I**, calculates the ANOVA table for a data file which has the number of factors (p) on the first line,

the levels $L_1\ L_2\ \ldots L_p$ on the second line, and then data values $Y_j(\mathbf{i})$ for $j = 1, 2, \ldots, n(\mathbf{i})$ one line per cell $\mathbf{i} = (i_1 i_2 \ldots i_p)$ with the lines in lexical order of the cells: $\mathbf{i}$=(1 1 $\ldots$1), (2 1 $\ldots$1), $\ldots$, ($L_1\ L_2, \ldots L_p$).

If $n[\mathbf{i}] \geq 1$ for all cells and $n[\mathbf{i}] > 1$ for some cell $\mathbf{i}$ then all interaction sums of squares are calculated. If $n[\mathbf{i}] = 1$ for all cells $\mathbf{i}$, the error sum of squares is calculated assuming $m_{12\cdots p}(\mathbf{i}) = 0$ for all $\mathbf{i}$ using $S_e^2 = S_{12\cdots p}^2$. To illustrate, the data of table 1 is entered as follows:

3		
4	3	2
1.11	0.97	
1.30	1.00	
1.22	1.13	
1.19	1.03	
1.09	0.99	
1.03	1.21	
1.34	1.41	
1.36	1.16	
1.21		
1.12	0.96	
1.34	1.19	
1.46	1.03	
1.52	1.45	
1.55	1.53	
1.38	1.08	
1.29		
1.27	1.22	
1.24	1.34	
1.40	1.21	
1.42	1.39	
1.24		
1.27		
1.46	1.39	
1.62		

← corresponding to →

p		
L_1	L_2	L_3
$Y[111][1]$	$Y[111][2]$	
$Y[211][1]$	$Y[211][2]$	
$Y[311][1]$	$Y[311][2]$	
$Y[411][1]$	$Y[411][2]$	
$Y[121][1]$	$Y[121][2]$	
$Y[221][1]$	$Y[221][2]$	
$Y[321][1]$	$Y[321][2]$	
$Y[421][1]$	$Y[421][2]$	
$Y[131][1]$		
$Y[231][1]$	$Y[231][2]$	
$Y[331][1]$	$Y[331][2]$	
$Y[431][1]$	$Y[431][2]$	
$Y[112][1]$	$Y[112][2]$	
$Y[212[1]$	$Y[212][2]$	
$Y[312][1]$	$Y[312][2]$	
$Y[412][1]$		
$Y[122][1]$	$Y[122][2]$	
$Y[222][1]$	$Y[222][2]$	
$Y[322][1]$	$Y[322][2]$	
$Y[422][1]$	$Y[422][2]$	
$Y[132][1]$		
$Y[232][1]$		
$Y[332][1]$	$Y[332][2]$	
$Y[432][1]$		

If we call the above file **multiway.data** and the C++ program **multiway.cpp** we can compile the C++ program under LINUX using the gnu C++ compiler as follows:

g++ -o multiway multiway.cpp

and then execute it with

multiway multiway.data

The program output is then

```
Do you want equal weights? Enter Y)es or N)o y:
Do you want to print out the data? Enter Y)es or N)o y:

Data:-a total of 43 observations. 3 factors with levels (4, 3, 2).
  j  cell      n(j)   Y.[j]    |  Y[j][k] for k=1,2,...,n[j]
-------------------------------------------------------------------
  1  (1,1,1)    2      1.0400  |      1.1100     0.9700
  2  (2,1,1)    2      1.1500  |      1.3000     1.0000
  3  (3,1,1)    2      1.1750  |      1.2200     1.1300
  4  (4,1,1)    2      1.1100  |      1.1900     1.0300
  5  (1,2,1)    2      1.0400  |      1.0900     0.9900
  6  (2,2,1)    2      1.1200  |      1.0300     1.2100
  7  (3,2,1)    2      1.3750  |      1.3400     1.4100
  8  (4,2,1)    2      1.2600  |      1.3600     1.1600
  9  (1,3,1)    1      1.2100  |      1.2100
 10  (2,3,1)    2      1.0400  |      1.1200     0.9600
 11  (3,3,1)    2      1.2650  |      1.3400     1.1900
 12  (4,3,1)    2      1.2450  |      1.4600     1.0300
 13  (1,1,2)    2      1.4850  |      1.5200     1.4500
 14  (2,1,2)    2      1.5400  |      1.5500     1.5300
 15  (3,1,2)    2      1.2300  |      1.3800     1.0800
 16  (4,1,2)    1      1.2900  |      1.2900
 17  (1,2,2)    2      1.2450  |      1.2700     1.2200
 18  (2,2,2)    2      1.2900  |      1.2400     1.3400
 19  (3,2,2)    2      1.3050  |      1.4000     1.2100
 20  (4,2,2)    2      1.4050  |      1.4200     1.3900
 21  (1,3,2)    1      1.2400  |      1.2400
 22  (2,3,2)    1      1.2700  |      1.2700
 23  (3,3,2)    2      1.4250  |      1.4600     1.3900
 24  (4,3,2)    1      1.6200  |      1.6200
```

ANALYSIS OF VARIANCE TABLE

Source	SS	D.F.	MS	F	P-value
Main Effects					
Factor (1)	0.0766	3	0.0255	1.5830	0.2264
Factor (2)	0.0100	2	0.0050	0.3102	0.7370
Factor (3)	0.3696	1	0.3696	22.9005	0.0001
2-way Interactions					
Factors (1,2)	0.2123	6	0.0354	2.1926	0.0893
Factors (1,3)	0.0810	3	0.0270	1.6723	0.2066
Factors (2,3)	0.0456	2	0.0228	1.4118	0.2681
3-way Interactions					
Factors (1,2,3)	0.0836	6	0.0139	0.8635	0.5389
Error	0.3066	19	0.0161		
Total	1.2429	42	0.0296		

14.5.2 Scheffé's Multiple Comparisons Method

When one of the main effect or interaction hypotheses is rejected, it is often of interest to explore reasons for rejections by exhibiting linear combinations of hypothesis parameter estimates that are significantly different from zero. See, for example the discussion in sections 3.4, 3.5 of Scheffé (1959) [8] We illustrate the method for the multifactor analysis of variance.

The estimate of the variance of the contrast (14.12) is

$$\widehat{Var}(\hat{\psi}_{12\ldots k}) = MS_e \sum_{i_1} \cdots \sum_{i_k} d^2(i_1, \ldots, i_k)/V_{12\ldots k}(i_1, \ldots, i_k)$$

where $MS_e = S_e^2/\nu_e$ is the error mean square estimate of σ^2 with

$$S_e^2 = \sum_{i_1} \cdots \sum_{i_p} \sum_j (Y_j(i_1, \ldots, i_p) - Y_{\cdot}(i_1, \ldots, i_p))^2, \quad \nu_e = N - L_1 L_2 \cdots L_p$$

[8] Scheffé, H. (1959) *The Analysis of Variance*, John Wiley and Sons, New York.

Table 14.5: Contrast coefficients $c(i_1, i_2)$ and corresponding $d(i_1, i_2)$.

$i_i i_2$	11	12	13	21	22	23	31	32	33	41	42	43
$c(i_1, i_2)$	1/2	-1/2	0	5/4	-1/4	-1	-1	1/2	1/4	-1	1/4	1
$d(i_1, i_2)$	9/16	-1/2	-1/16	21/16	-1/4	-17/16	-41/48	7/12	13/48	-49/48	1/6	41/48

and $N = n(+, +, \ldots, +)$ is the total number of observations. Scheffé (1959,page 69) proves that the probability is $1-\alpha$ that the values of all contrasts simultaneously satisfy the inequalities

$$\hat{\psi}_{12\ldots k} - h \times (\widehat{Var}(\hat{\psi}_{12\ldots k}))^{1/2} \leq \psi_{12\ldots k} \leq \hat{\psi}_{12\ldots k} + h \times (\widehat{Var}(\hat{\psi}_{12\ldots k}))^{1/2}$$

where $\nu_{12\ldots k} = (L_1 - 1)(L_2 - 1) \cdots (L_k - 1)$ is the numerator degrees of freedom and the constant $h = (\nu_{12\ldots k} F_{\alpha,\nu_{12\ldots k},\nu_e})^{1/2}$ for the hypothesis $H_{12\ldots k}$ and $F_{\alpha,\nu_{12\ldots k},\nu_e}$ is the upper α probability point for the F distribution with degrees of freedom $\nu_{12\ldots k}$ and ν_e.

The values of $V_{12\ldots k}$ and MS_e have previously been calculated for the ANOVA table. It remains to calculate the contrast coefficients $d(i_1, \ldots, i_k)$ for $c(i_1, \ldots, i_k)$.

To illustrate a calculation for the previous example, consider the interactions $m_{12}(i_1, i_2)$ which are significantly different from zero at the 10% significance level (P-value 0.0893). Table 5 gives least square estimates

$$\hat{m}_{12}(i_1, i_2) = Y_{\cdot}(i_1, i_2, \cdot) - Y_{\cdot}(i_1, \cdot, \cdot) - Y_{\cdot}(\cdot, i_2, \cdot) + Y_{\cdot}(\cdot, \cdot, \cdot) \ .$$

Table 5. m_{12} interaction estimates.

$\hat{m}_{12}(i_1, i_2)$	$i_2 = 1$	2	3
$i_1 = 1$	0.065625	-0.056875	-0.008750
2	0.123125	-0.019375	-0.103750
3	-0.080208	0.054792	0.025417
4	-0.108542	0.021458	0.087083

After some trial and error on the choice of coefficients $c(i_1, i_2)$ the coefficients in table 6 were found to yield a linear combination significantly different from zero for the 90% confidence interval.

We have the value of the 90% confidence interval

$$\hat{\psi}_{12} - h(\widehat{Var}(\hat{\psi}_{12}))^{1/2} \leq \psi_{12} \leq \hat{\psi}_{12} + h(\widehat{Var}(\hat{\psi}_{12}))^{1/2}$$

$$= 0.638698 - (19 \times 2.10936)^{1/2}(0.031800)^{1/2} \leq \psi_{12} \leq$$
$$0.638698 + (19 \times 2.10936)^{1/2}(0.031800)^{1/2}$$
$$= 0.00429 \leq \psi_{12} \leq 1.27310$$

does not contain zero ($F_{0.10,6,19} = 2.10936$).

14.6 Analysis of Covariance

Consider the model

$$\tilde{\Omega}: \quad \mathbf{Y}^{n\times 1} = \mathbf{U}^{n\times r}\boldsymbol{\gamma}^{r\times 1} + \mathbf{V}^{n\times s}\boldsymbol{\delta}^{s\times 1} + \boldsymbol{\varepsilon}^{n\times 1}$$

where $\boldsymbol{\varepsilon}$ is multivariate normal $\mathcal{N}_n(\mathbf{0}, \sigma^2\mathbf{I}_n)$ for the $n \times n$ identity matrix $\mathbf{I}_n$ with γ, δ, and σ unknown and $n > r + s$, with $r + s$ the rank of $(\mathbf{U}, \mathbf{V})$. The parameters δ are covariates with $\mathbf{V}$ known. Hypotheses of interest are

$$H_{\tilde{\omega}}: \ \mathbf{B}_0^{m\times r}\boldsymbol{\gamma} = \mathbf{c}_0^{m\times 1}$$

where $\mathbf{B}_0$ and $\mathbf{c}_0$ are given.

If we write $\mathbf{X} = (\mathbf{U}, \mathbf{V})$, $\boldsymbol{\beta}^T = (\boldsymbol{\gamma}^T, \boldsymbol{\delta}^T)$, $p = r + s$, and $\mathbf{A}_0^{m\times p} = (\mathbf{B}_0^{m\times r}, \mathbf{0}^{m\times s})$ then the previous linear model (14.1) applies with $\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}}$ and $\hat{\boldsymbol{\delta}}_{\tilde{\Omega}}$ satisfying

$$\mathbf{X}^T\mathbf{X}\hat{\boldsymbol{\beta}}_{\tilde{\Omega}} = \mathbf{X}^T\mathbf{Y}$$

or

$$\mathbf{U}^T\mathbf{U}\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}} + \mathbf{U}^T\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} = \mathbf{U}^T\mathbf{Y}$$
$$\mathbf{V}^T\mathbf{U}\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}} + \mathbf{V}^T\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} = \mathbf{V}^T\mathbf{Y}$$

Solving, we obtain

$$\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}} = (\mathbf{U}^T\mathbf{U})^{-1}(\mathbf{U}^T\mathbf{Y} - \mathbf{U}^T\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}}) \ .$$

If we write the model

$$\Omega: \quad \mathbf{Y}^{n\times 1} = \mathbf{U}\boldsymbol{\gamma} + \boldsymbol{\varepsilon}$$

then following Scheffé (page 204)[9], we can express the sum of squares for $\tilde{\Omega}$ in terms of the sums of squares for Ω.

[9] Scheffé, H. (1959) *The Analysis of Variance*, John Wiley and Sons, New York.

Define

$$\begin{aligned}\mathbf{P}(\tilde{\Omega})\mathbf{Y} &= \mathbf{U}\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}} + \mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} \\ &= \mathbf{U}(\mathbf{U}^T\mathbf{U})^{-1}\mathbf{U}^T\mathbf{Y} + (\mathbf{I} - \mathbf{U}(\mathbf{U}^T\mathbf{U})^{-1}\mathbf{U})\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} \\ &= \mathbf{P}(\Omega)\mathbf{Y} + \mathbf{Q}(\Omega)\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}}\end{aligned}$$

where

$$\mathbf{P}(\Omega) = \mathbf{U}(\mathbf{U}^T\mathbf{U})^{-1}\mathbf{U}, \text{ and } \mathbf{Q}(\Omega) = \mathbf{I} - \mathbf{U}(\mathbf{U}^T\mathbf{U})^{-1}\mathbf{U}\ .$$

Then using

$$||\mathbf{Z}||^2 = \mathbf{Z}^T\mathbf{Z}, \quad \mathbf{Q}(\Omega)^T\mathbf{Q}(\Omega) = \mathbf{Q}(\Omega), \quad \text{and } \mathbf{V}^T\mathbf{Q}(\Omega)\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} = \mathbf{V}^T\mathbf{Q}(\Omega)\mathbf{Y}$$

we have

$$\begin{aligned}S_e^2(\tilde{\Omega}) &= ||\mathbf{Y} - \mathbf{P}(\tilde{\Omega})\mathbf{Y}||^2 \\ &= ||\mathbf{Y} - \mathbf{P}(\Omega)\mathbf{Y} - \mathbf{Q}(\Omega)\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}}||^2 \\ &= ||\mathbf{Y} - \mathbf{P}(\Omega)\mathbf{Y}||^2 - 2\mathbf{Y}^T(\mathbf{I} - \mathbf{P}(\Omega))\mathbf{Q}(\Omega)\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} + || + ||\mathbf{Q}(\Omega)\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}}||^2 \\ &= S_e^2(\Omega) - \hat{\boldsymbol{\delta}}_{\tilde{\Omega}}^T\mathbf{V}^T\mathbf{Q}(\Omega)\mathbf{Y}\ .\end{aligned}$$

If we write

$$\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} = \begin{pmatrix} \hat{\delta}_{1\tilde{\Omega}} \\ \hat{\delta}_{2\tilde{\Omega}} \\ \vdots \\ \hat{\delta}_{s\tilde{\Omega}} \end{pmatrix} \text{ and } \mathbf{V} = (\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_s) \text{ where } \mathbf{v}_j = \begin{pmatrix} v_{1j} \\ v_{2j} \\ \vdots \\ v_{nj} \end{pmatrix}$$

then with $S_e^2(\Omega) = \mathbf{Y}^T\mathbf{Q}(\Omega)\mathbf{Y}$ we have

$$S_e^2(\tilde{\Omega}) = S_e^2(\Omega) - \sum_{j=1}^{s} \hat{\delta}_{j\tilde{\Omega}}\mathbf{v}_j^T\mathbf{Q}(\Omega)\mathbf{Y} \tag{14.20}$$

and

$$\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} = (\mathbf{V}^T\mathbf{Q}(\Omega)\mathbf{V})^{-1}\mathbf{V}^T\mathbf{Q}(\Omega)\mathbf{Y}\ .$$

For calculating the numerator sum of squares for the hypothesis $H_{\tilde{\omega}}$ we can use equation (14.1)

$$S_{H_{\tilde{\omega}}}^2 = S^2(\tilde{\omega}) - S^2(\tilde{\Omega}) = (\mathbf{A}_0\hat{\boldsymbol{\beta}}_{\tilde{\Omega}} - \mathbf{c}_0)^T(\mathbf{A}_0(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{A}_0^T)^{-1}(\mathbf{A}_0\hat{\boldsymbol{\beta}}_{\tilde{\Omega}} - \mathbf{c}_0)$$

$$= (\mathbf{B}_0\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}} - \mathbf{c}_0)^T(\mathbf{B}_0(\mathbf{U}^T\mathbf{R}\mathbf{U})^{-1}\mathbf{B}_0^T)^{-1}(\mathbf{B}_0\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}} - \mathbf{c}_0)$$

where $\mathbf{R} = \mathbf{I} - \mathbf{V}(\mathbf{V}^T\mathbf{V})^{-1}\mathbf{V}^T$ and $\hat{\boldsymbol{\gamma}}_{\tilde{\Omega}} = (\mathbf{U}^T\mathbf{R}\mathbf{U})^{-1}\mathbf{U}^T\mathbf{R}\mathbf{Y}$.

If we consider the model Ω and the hypothesis $H_\omega:\ \mathbf{B}_0\boldsymbol{\gamma} = \mathbf{c}_0$ and we find that $S^2(\omega)$ is a quadeatic form $\mathbf{Y}\mathbf{Q}(\omega)\mathbf{Y}$, which is the case when $\mathbf{c}_0 = \mathbf{0}$, then we can also calculate the numerator sum of squares $S^2_{H_{\tilde{\omega}}} = S^2(\tilde{\omega}) - S^2(\tilde{\Omega})$ using equation (14.20) and

$$S^2(\tilde{\omega}) = S^2(\tilde{\Omega}) - \sum_{j=1}^{s} \hat{\delta}_{j\tilde{\omega}}\mathbf{v}_j^T\mathbf{Q}(\omega)\mathbf{Y}\ .$$

Here the vector $\hat{\boldsymbol{\delta}}_{\tilde{\omega}}$ (as well as $\hat{\boldsymbol{\gamma}}_{\tilde{\omega}}$) minimizes

$$||\mathbf{Y} - \mathbf{U}\boldsymbol{\gamma} - \mathbf{V}\boldsymbol{\delta}||^2 \text{ subject to } \mathbf{B}_0\boldsymbol{\gamma} = \mathbf{c}_0$$

or

$$\hat{\boldsymbol{\delta}}_{\tilde{\omega}} = (\mathbf{V}^T\mathbf{Q}(\omega)\mathbf{V})^{-1}\mathbf{V}^T\mathbf{Q}(\omega)\mathbf{Y}$$

14.6.1 An Example

For an example, consider the balanced two-way layout with two covariates:

$$\tilde{\Omega}: \quad Y_{jkl} = \mu_{jk} + v_{jkl}^{(1)}\delta_1 + v_{jkl}^{(2)}\delta_2 + \varepsilon_{jkl}$$

for $j = 1, 2, \ldots, J$, $k = 1, 2, \ldots, K$, and $l = 1, 2, \ldots, L$ with independent $\varepsilon_{jkl}:\ \mathcal{N}(0, \sigma^2)$.

Write

$$\alpha_j^{(1)} = \mu_{j\cdot} - \mu_{\cdot\cdot}, \quad \alpha_k^{(2)} = \mu_{\cdot k} - \mu_{\cdot\cdot}, \quad \alpha_{jk}^{(12)} = \mu_{jk} - \mu_{j\cdot} - \mu_{\cdot k} + \mu_{\cdot\cdot}$$

and consider the hypotheses

$$H_1:\ \alpha_j^{(1)} = 0 \text{ for all } j = 1, 2, \ldots, J,$$

$$H_2:\ \alpha_k^{(2)} = 0 \text{ for all } k = 1, 2, \ldots, K,$$

$$H_{12}:\ \alpha_{jk}^{(12)} = 0 \text{ for all } j = 1, 2, \ldots, J,\ k = 1, 2, \ldots, K\ .$$

From equations (14.3) and (14.4) we have

$$S^2_{H_1}(\omega) = KL\sum_{j=1}^{J}(Y_{j\cdot\cdot} - Y_{\cdot\cdot\cdot})^2$$

and

$$S_e^2(\Omega) = \sum_{j=1}^{J}\sum_{k=1}^{K}\sum_{l=1}^{L}(Y_{jkl} - Y_{jk\cdot})^2 = \mathbf{Y}^T\mathbf{Q}(\Omega)\mathbf{Y}$$

$$S^2(\omega_1) = S_e^2(\Omega) + S_{H_1}^2(\omega) = \mathbf{Y}^T\mathbf{Q}(\omega_1)\mathbf{Y}$$

$$= \sum_{j=1}^{J}\sum_{k=1}^{K}\sum_{l=1}^{L}(Y_{jkl} - Y_{jk\cdot})^2 + KL\sum_{j=1}^{J}(Y_{j\cdot\cdot} - Y_{\cdot\cdot\cdot})^2 \ .$$

Then

$$S_e^2(\tilde{\Omega}) = S_e^2(\Omega) - \hat{\delta}_{1\tilde{\Omega}}\mathbf{v}^{(1)}\mathbf{Q}(\Omega)\mathbf{Y} - \hat{\delta}_{2\tilde{\Omega}}\mathbf{v}^{(2)}\mathbf{Q}(\Omega)\mathbf{Y}$$

where, in lexical order,

$$\mathbf{Y}^T = (Y_{111}, Y_{112}, \cdots, Y_{11L}, Y_{121}, \cdots, Y_{12L}, \cdots, Y_{JK1}, \cdots, Y_{JKL})$$

and

$$(\mathbf{v}^{(i)})^T = \left(v_{111}^{(i)}, v_{112}^{(i)}, \cdots, v_{11L}^{(i)}, v_{121}^{(i)}, \cdots, v_{12L}^{(i)}, \cdots, v_{JK1}^{(i)}, \cdots, v_{JKL}^{(i)}\right) \text{ for } i = 1, 2 \ .$$

The covariate parameter estimates are obtained as solutions to the symmetric linear equations

$$\mathbf{V}^T\mathbf{Q}(\Omega)\mathbf{V}\hat{\boldsymbol{\delta}}_{\tilde{\Omega}} = \mathbf{V}^T\mathbf{Q}(\Omega)\mathbf{Y}$$

or

$$\begin{pmatrix} (\mathbf{v}^{(1)})^T\mathbf{Q}(\Omega)\mathbf{v}^{(1)} & (\mathbf{v}^{(1)})^T\mathbf{Q}(\Omega)\mathbf{v}^{(2)} \\ (\mathbf{v}^{(2)})^T\mathbf{Q}(\Omega)\mathbf{v}^{(1)} & (\mathbf{v}^{(2)})^T\mathbf{Q}(\Omega)\mathbf{v}^{(2)} \end{pmatrix} \begin{pmatrix} \hat{\delta}_{1,\tilde{\Omega}} \\ \hat{\delta}_{2,\tilde{\Omega}} \end{pmatrix} = \begin{pmatrix} (\mathbf{v}^{(1)})^T\mathbf{Q}(\Omega)\mathbf{Y} \\ (\mathbf{v}^{(2)})^T\mathbf{Q}(\Omega)\mathbf{Y} \end{pmatrix}$$

Similarly,

$$S^2(\tilde{\omega}_1) = S^2(\omega_1) - \hat{\delta}_{1\tilde{\omega}_1}\mathbf{v}^{(1)}\mathbf{Q}(\omega_1)\mathbf{Y} - \hat{\delta}_{2\tilde{\omega}_1}\mathbf{v}^{(2)}\mathbf{Q}(\omega_1)\mathbf{Y}$$

with the hypothesis covariate estimates solutions to

$$\begin{pmatrix} (\mathbf{v}^{(1)})^T\mathbf{Q}(\omega)\mathbf{v}^{(1)} & (\mathbf{v}^{(1)})^T\mathbf{Q}(\omega)\mathbf{v}^{(2)} \\ (\mathbf{v}^{(2)})^T\mathbf{Q}(\omega)\mathbf{v}^{(1)} & (\mathbf{v}^{(2)})^T\mathbf{Q}(\omega)\mathbf{v}^{(2)} \end{pmatrix} \begin{pmatrix} \hat{\delta}_{1,\tilde{\omega}} \\ \hat{\delta}_{2,\tilde{\omega}} \end{pmatrix} = \begin{pmatrix} (\mathbf{v}^{(1)})^T\mathbf{Q}(\omega)\mathbf{Y} \\ (\mathbf{v}^{(2)})^T\mathbf{Q}(\omega)\mathbf{Y} \end{pmatrix} \ .$$

Then

$$S_{H_1}^2(\tilde{\omega}_1) = S^2(\tilde{\omega}_1) - S_e^2(\tilde{\Omega}) \ .$$

The $\mathcal{F}$ statistic is then

$$\mathcal{F} = \frac{S^2_{H_1}(\tilde{\omega_1})/(J-1)}{S^2_e(\tilde{\Omega})/(JK(L-1)-2)}$$

which has the $F_{(J-1),JK(L-1)-2}$ distribution.

A Pascal program that calculates the analysis of covariance (ANCOVA) table for multifactor designs with P-values is given by Shu-Yen Ho[10]

14.7 Problems

1. Let

$$Y_{jklm} = \mu + \alpha_j + \beta_k + \gamma_l + \delta_{jk} + \eta_{jl} + \xi_{kl} + \lambda_{jkl} + \varepsilon_{jklm}$$

for $j = 1, 2, \ldots, J,\ k = 1, 2, \ldots, K,\ l = 1, 2, \ldots, L,\ m = 1, 2, \ldots, M$ where $\varepsilon_{jklm} : \mathcal{N}(0, \sigma^2)$ are independent and

$$\sum_{j=1}^{J} \alpha_j = \sum_{k=1}^{K} \beta_k = \sum_{l=1}^{L} \gamma_l = 0,$$

$$\sum_{j=1}^{J} \delta_{jk} = \sum_{k=1}^{K} \delta_{jk} = \sum_{j=1}^{J} \eta_{jl} = \sum_{l=1}^{L} \eta_{jl} = \sum_{k=1}^{K} \xi_{kl} = \sum_{l=1}^{L} \xi_{kl} = 0$$

$$\sum_{j=1}^{J} \lambda_{jkl} = \sum_{k=1}^{K} \lambda_{jkl} = \sum_{l=1}^{L} \lambda_{jkl} = 0\ .$$

Derive closed form expressions for sums of squares in the ANOVA table for testing main effects and higer order interactions are zero. Give expressions for Scheffé's method of multiple comparisons to explain any effects significantly different from zero.

[10] Ho, Shu-Yen (1990). *Sparse Matrix Methods for the Unbalanced Multifactor ANCOVA.* University of Wisconsin at Madison Ph.D. Thesis, Department of Statistics. See also S.H.Ho and J.H. Klotz (1992). Sparse matrix methods for unbalanced multifactor analysis of variance and covariance. *Journal of Statistical Computation and Simulation* **41** 55-72.

2. Let

$$Y_{jklm} = \mu + \alpha_j + \beta_k + \gamma_l + \delta_{jk} + \eta_{jl} + \xi_{kl} + \lambda_{jkl} + \rho t_{jklm} + \phi u_{jklm} + \varepsilon_{jklm}$$

with side conditions and errors ε_{jklm} as in problem 1 and t_{jklm}, u_{jklm} given. Give formulae for the ANCOVA table for testing main effects and higer order interactions are zero.

3. Consider the following linear model

$$Y_i = \beta_0 + \beta_1 c_{1i} + \beta_2 x_{2i} + \beta_3 x_{3i} + \varepsilon_i \text{ for } i = 1, 2, \ldots, n$$

with ε_i independent $\mathcal{N}(0, \sigma^2)$ for the data

i	x_{1i}	x_{2i}	x_{3i}	Y_i
1	1.0	2.0	1.5	12
2	1.5	2.0	2.1	13
3	1.0	3.7	0.9	25
4	2.5	0.3	6.0	18
5	0.5	2.5	4.0	17
6	0.8	3.0	6.5	20

Test the hypothesis $H: \ \beta_1 + \beta_3 = 0$ versus $A: \ \beta_1 + \beta_3 \neq 0$ and give a 90% confidence interval for $\beta_1 + \beta_3$.

Chapter 15

Nonparametric Methods

Nonparametric or distribution free methods are designed to make inferences with few assumptions on the underlying distribution of the observations. Instead of a parametric model, for example $\mathcal{N}(\mu, \sigma^2)$, minimal assumptions such as $X_1, X_2, \ldots, X_n$ are independent with distribution $F(x)$ continuous are considered.

15.1 The Sign Test

One of the simplest nonparametric methods is the sign test. Assume that $X_1, X_2, \ldots, X_n$ are independent with c.d.f. $F(x)$ with median m. That is m is a value such that

$$P[X_i \leq m] = F(m) \geq \frac{1}{2} \leq 1 - F(m^-) = P[X_i \geq m]$$

where $F(m^-) = \lim_{\varepsilon \downarrow 0} F(m - \varepsilon)$ If F is continuous then $F(m) = \frac{1}{2}$. We consider one-sided hypotheses

$$H_1^* : \ m \leq m_0 \text{ vs } A_1^* : \ m > m_0$$

$$H_2^* : \ m \geq m_0 \text{ vs } A_2^* : \ m < m_0$$

or the two-sided hypothesis

$$H_{12}^* : \ m = m_0 \text{ vs } A_{12}^* : \ m \neq m_0 \ .$$

Consider the statistics

$$S_+ = \sum_{i=1}^{n} I[X_i > m_0], \quad S_0 = \sum_{i=1}^{n} I[X_i = m_0], \text{ and } S_- = \sum_{i=1}^{n} I[X_i < m_0]$$

which are the number of observations that exceed, equal, or are less than m_0. The joint distribution of (S_+, S_0, S_-) is that of the multinomial

$$P[S_+ = s_+, S_0 = s_0, S_- = n - s_+ - s_0] = \frac{n!}{s_+! s_0! (n - s_+ - s_0)!} p_+^{s_+} p_0^{s_0} p_-^{(n-s_+-s_0)}$$

where

$$p_+ = P[X_i > m_0], \quad p_0 = P[X_i = m_0], \text{ and } p_- = P[X_i < m_0] = 1 - p_+ - p_0 \ .$$

We consider the hypotheses

$$H_1 : \ p_+ \le p_-, \quad H_2 : \ p_+ \ge p_-, \text{ and } H_{12} : \ p1 = p_2$$

and the corresponding alternatives

$$A_1 : \ p_+ > p_-, \quad A_2 : \ p_+ < p_-, \text{ and } A_{12} : \ p1 \ne p_2 \ .$$

$H_1 \Longrightarrow H_1^*$

$p_+ \le p_-$ gives $p_+ + p_- \le 2p_-$ or $1 - p_0 \le 2p_-$. Thus $p_- \ge (1 - p_0)/2$ and $P[X_i \le m_0] = p_- + p_0 \ge (1 - p_0)/2 + p_0 \ge 1/2$ and $m \le m_0$.

$H_2 \Longrightarrow H_2^*$

$p_+ \ge p_-$ gives $p_+ \ge (1 - p_0)/2$ and $P[X_i \ge m_0] = p_+ + p_0 \ge (1 - p_0)/2 + p_0 \ge 1/2$ and $m \ge m_0$.

$H_{12} \Longrightarrow H_{12}^*$

$p_+ = p_-$ gives $2p_+ + p_0 = 1 = 2p_- + p_0$ or $p_+ = (1 - p_0)/2 = p_-$. Then $P[X_i \ge m_0] = p_+ + p_0 = (1 - p_0)/2 + p_0 \ge 1/2 <= p_- + p_0 = P[X_i \le m_0]$ and $m = m_0$.

If F is continuous, so that $p_0 = 0$ then the hypotheses H are equivalent to the H^* hypotheses.

To eliminate the nuisance parameter p_0 we condition on S_0. When $p_+ = p_-$, then $p_+/(1 - p_0) = 1/2$ and

$$P_H[S_+ = s_+ | S_0 = s_0] = \frac{n! p_+^{s_+} p_0^{s_0} p_+^{(n-s_+-s_0)}}{s_+! s_0! (n - s_+ - s_0)!} / \binom{n}{s_0} p_0^{s_0} (1 - p_0)^{(n-s_0)}$$

$$= \binom{n-s_0}{s_+} \frac{1}{2^{n-s_0}} \ .$$

For the one-sided composite hypotheses, we use a least favorable distribution that puts probability one for $p_+ = p_-$.

For testing H_1 versus A_1 we reject H_1 in favor of A_1 if $S_+ \geq C_1$, given $S_0 = s_0$, where the type I error α and C_1 satisfy

$$\sum_{x=C_1}^{n-s_0} \binom{n-s_0}{x} \frac{1}{2^{(n-s_0)}} = \alpha \ . \tag{15.1}$$

The power of the test for H_1 is given for the alternative $A_1 : \ p_+ > p_-$ by

$$\gamma = \sum_{x=C_1}^{n-s_0} \binom{n-s_0}{x} \left(\frac{p_+}{1-p_0}\right)^x \left(\frac{p_-}{1-p_0}\right)^{n-s_0-x} \ .$$

For testing H_2 versus A_2, given $S_0 = s_0$, we reject if $S_+ \leq C_2$ where α and C_2 satisfy

$$\sum_{x=0}^{C_2} \binom{n-s_0}{x} \frac{1}{2^{(n-s_0)}} = \alpha \ . \tag{15.2}$$

For the two-sided hypothesis, given $S_0 = s_0$, we reject H_{12} in favor of A_{12} if $S_+ \leq C_{12}$ or $S_+ \geq n - s_0 - C_{12}$ where

$$\sum_{x=0}^{C_{12}} \binom{n-s_0}{x} \frac{1}{2^{(n-s_0)}} = \alpha/2 \ .$$

15.1.1 Confidence Interval for the Median

We consider the case where the distribution $F(x) = G(x-m)$ where G is continuous with $G(0) = 1/2$ so that m is the median of F. The acceptance region for the two-sided test based on $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ in this continuous distribution case is

$$\mathcal{A}(m_0) = \{\mathbf{X} : C_{12} < S_+ < n - C_{12}\}$$

where

$$\sum_{x=0}^{C_{12}} \binom{n}{x} \frac{1}{2^n} = \alpha/2 \ . \tag{15.3}$$

The associated confidence set for m with confidence coefficient $1-\alpha$ is

$$\mathcal{S}(\mathbf{X}) = \{m : C_{12} < S_+(m) < n - C_{12}\}$$

where $S_+(m) = \sum_{i=1}^n I[X_i > m]$.

To simplify the confidence set, let $X_{(1)} \le X_{(2)} \le \ldots \le X_{(n)}$ be the order statistics. Then $X_{(r)} \le m$ if and only if $S_+(m) \le n - r$ and

$$\mathcal{S}(\mathbf{X}) = \{m : C_{12} < S_+(m) < n - C_{12}\} = \{m : C_{12} < S_+(m) \le n - C_{12} - 1\}$$

$$= \{m : S_+(m) \le C_{12}\}^c \cap \{m : S_+(m) \le n - C_{12} - 1\}$$

$$= \{m : X_{(n-C_{12})} \le m\}^c \cap \{m : X_{(C_{12}+1)} \le m\}$$

$$= \{m : X_{(C_{12}+1)} \le m < X_{(n-C_{12})}) = [X_{(C_{12}+1)}, X_{(n-C_{12})})$$

Corresponding one-sided confidence bounds for the median m, with confidence coefficient $1-\alpha$, are

$$\{m : X_{(n-C_1+1)} \le m\}, \text{ and } \{m : m < X_{(n-C_2)}\}$$

for the lower and upper bounds. Here C_1, C_2, and C_{12} satisfy equations (15.1), (15.2), and (15.3) with $s_0 = 0$.

15.1.2 Point Estimate for the Median

If the sample size is odd ($n = 2r+1$) then the 50% upper confidence bound for the median is $(-\infty, X_{(r+1)})$ since $(-\infty, X_{(n-C_2)})$ is the upper bound where from equation (15.2)

$$\sum_{x=0}^{C_2} \binom{2r+1}{x} \frac{1}{2^{2r+1}} = 0.5$$

and $C_2 = r$ so that $n - C_2 = 2r + 1 - r = r + 1$. Similarly the 50% lower confidence bound is $[X_{(r+1)}, \infty)$ and it seems reasonable to take the point estimate for m to be $X_{(r+1)}$ =median$(X_1, X_2, \ldots, X_n)$. For even sample size ($n = 2r$) the upper bound with confidence coefficient at least 50% and closest to it is $(-\infty, X_{(r)})$ since

$$\sum_{x=0}^{r} \binom{2r}{x} \frac{1}{2^{2r}} > \frac{1}{2} > \sum_{x=0}^{r-1} \binom{2r}{x} \frac{1}{2^{2r}} .$$

To prove this

$$\sum_{x=0}^{r} \binom{2r}{x} \frac{1}{2^{2r}} = \sum_{x=0}^{r} \binom{2r}{2r-x} \frac{1}{2^{2r}} = \sum_{u=r}^{2r} \binom{2r}{u} \frac{1}{2^{2r}} \ .$$

So

$$2\sum_{x=0}^{r} \binom{2r}{x} \frac{1}{2^{2r}} = \sum_{x=0}^{r} \binom{2r}{x} \frac{1}{2^{2r}} + \sum_{u=r}^{2r} \binom{2r}{u} \frac{1}{2^{2r}} = 1 + \binom{2r}{r} \frac{1}{2^{2r}} \ .$$

Dividing by 2 we get

$$\sum_{x=0}^{r} \binom{2r}{x} \frac{1}{2^{2r}} = \frac{1}{2} + \binom{2r}{r} \frac{1}{2^{2r+1}} > \frac{1}{2} \ .$$

A similar proof shows

$$\sum_{x=0}^{r-1} \binom{2r}{x} \frac{1}{2^{2r}} = \frac{1}{2} - \binom{2r}{r} \frac{1}{2^{2r+1}} < \frac{1}{2} \ .$$

Thus $C_2 = r$, $n - C_2 = 2r - r = r$ and $(-\infty, X_{(r)})$ is the upper bound with confidence coefficient

$$\frac{1}{2} + \binom{2r}{r} \frac{1}{2^{2r+1}} \ .$$

Similarly, $[X_{(r+1)}, \infty)$ is the lower bound with the same confidence coefficient. We average these two bounds to get the point estimate

$$\frac{X_{(r)} + X_{(r+1)}}{2} = \tilde{X} = \text{median}(X_1, X_2, \ldots, X_n) \ .$$

In both cases it is the median of the sample.

To calculate the binomial probability we can use the incomplete beta c.d.f. with the identity

$$\sum_{k=0}^{x} \binom{n}{k} \frac{1}{2^n} = I_{1/2}(n-x, x+1)$$

and use the subroutine in **cdf.h**, **Appendix A**.

15.1.3 Small Sample Performance Comparisons

We compare the performance of the sign test with that of parametric tests. Consider first the $\mathcal{N}(\mu, \sigma^2)$ distribution where σ^2 is known. Here the median $m = \mu$ and we test $H_1 : \ \mu \leq \mu_0$ versus $A_1 : \ \mu > \mu_0$. The parametric $\bar{X}$ test based on n_2 observations rejects H_1 in favor of A_1 if

$$Z = \frac{\sqrt{n_2}(\bar{X} - \mu_0)}{\sigma} \geq z_\alpha$$

where

$$\alpha = 1 - \Phi(z_\alpha), \quad \Phi(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-t^2/2} dt \ .$$

A measure of efficiency of the sign test based on n_1 observations relative to the $\bar{X}$ test based on n_2 observations is $e_{12}(\alpha, \beta, n_1) = n_2/n_1$. Here the sample sizes are chosen for a fixed alternative μ so that the type I error α and type II error β are the same for each test. The problem with this definition is that the sample size is a discrete variable and it is often impossible to exactly match both error probabilities. If we choose a sample size n_1 and a critical value C_1 that gives type I error for the sign test $\alpha_{S_+} = \alpha$ then we can adjust z_α so that the type I error for the $\bar{X}$ test satisfies $\alpha_{\bar{X}} = \alpha$. However it may not be possible to adjust n_2 so that $\beta_{\bar{X}} = \beta_{S_+} = \beta$. It is possible to find integers $n_2^* < n_2^{**}$ such that

$$\Phi(z_\alpha - \sqrt{n_2^{**}}(\mu - \mu_0)/\sigma) \leq \beta \leq \Phi(z_\alpha - \sqrt{n_2^*}(\mu - \mu_0)/\sigma) \ .$$

Thus we need some kind of interpolation between n_2^*, n_2^{**} to define n_2. In this example, the easiest interpolation is to pretend n_2 is a continuous variable with

$$\Phi(z_\alpha - \sqrt{n_2}(\mu - \mu_0)/\sigma) = \beta \ .$$

Solving, we obtain

$$n_2 = \left[\frac{(z_\alpha + z_\beta)\sigma}{\mu} \right]^2$$

For example, with $n_1 = 50$, $C_1 = 30$,

$$\alpha_{S_+} = \sum_{x=30}^{50} \binom{50}{x} \frac{1}{2^{50}} \doteq 0.10319 \ .$$

Table 15.1: Efficiency of the sign test relative to the $\bar{X}$ test.

n_1	α	β	μ	n_2	e_{12}
11	0.1133	0.1013	0.9542	6.771	0.616
16	0.1051	0.1188	0.7722	9.935	0.621
23	0.1050	0.1177	0.6434	14.39	0.626
50	0.1013	0.1156	0.4399	31.55	0.631
76	0.1034	0.1105	0.3585	48.12	0.633
106	0.1032	0.1073	0.3055	67.24	0.634
125	0.1052	0.1085	0.2793	79.33	0.634
150	0.1103	0.1061	0.2534	95.08	0.634

For $\mu_0 = 0$, $\mu = 0.43991$, $\sigma^2 = 1$, we have $p_+ = 1 - \Phi(\mu_0 - \mu) \doteq \Phi(0.43991) \doteq 0.67$ and

$$\beta_{S_+} \doteq \sum_{x=0}^{29} \binom{50}{x} (0.67)^x (0.33)^{50-x} \doteq 0.115641 \ .$$

Then

$$z_\alpha = \Phi^{-1}(1 - 0.101319) \doteq 1.27407, \quad z_\beta \doteq \Phi^{-1}(1 - 0.115641) = 1.19706$$

$$n_2 = \left[\frac{1.27407 + 1.19706}{0.43991}\right]^2 \doteq 31.5547, \text{ and } e_{12} \doteq 31.5547/50 \doteq 0.63109 \ .$$

Table 15.1 gives additional such efficiency values.

Thus the nonparametric test relative to the parametric test requires about a 37% larger sample size for the protection against the parametric model not being valid in this example.

15.1.4 Large Sample Performance Comparisons

As the sample sizes get large, it is also of interest to compare nonparametric and parametric tests. We look at asymptotic efficiency as $n_1 \to \infty$ with $\alpha_{S_+}(n_1) \to \alpha$ and $\beta_{S_+}(n_1) \to \beta$ where $0 < \alpha, \beta < 1$.

Using the central limit theorem for the binomial distribution we must have $C_1 = C_1(n_1)$ satisfying

$$\frac{(C_1(n_1) - n_1/2)}{\sqrt{n_1/4}} \longrightarrow z_\alpha = \Phi^{-1}(1-\alpha) \tag{15.4}$$

with $-\infty < z_\alpha < \infty$ since $0 < \alpha < 1$.

Next, for $n_1 \to \infty$, $\alpha_{S_+}(n_1) \to \alpha$, in order for $\beta_{S_+}(n_1) \to \beta$ with $0 < \alpha, \beta < 1$ we must have the alternative $\mu = \mu_{n_2} \to \mu_0$ since if not there would be a subsequence converging to a limit value for μ greater than μ_0. Because the $\bar{X}$ test is consistent, we would have $\beta_{\bar{X}} \to 0$ for this subsequence contradicting $\beta_{\bar{X}}(n_2) \to \beta > 0$. This also implies

$$p_+ = \Phi((\mu_{n_2} - \mu_0)/\sigma) \to 1/2$$

using the continuity of $\Phi(x)$.

Using the normal approximation to the binomial under the alternative, the Berry-Esseen approximation (9.1) gives

$$\left|\beta_{S_+}(n_1) - \Phi\left(\frac{C_1(n_1) - n_1 p_+}{\sqrt{n_1 p_+(1-p_+)}}\right)\right| \le K\frac{((1-p_+)^3 p_+ + p_+^3(1-p_+))}{\sqrt{n_1 p_+(1-p_+)}} \longrightarrow 0$$

and since $\beta_{S_+}(n_1) \to \beta$ where $0 < \beta < 1$ we have

$$\Phi\left(\frac{C_1(n_1) - n_1 p_+}{\sqrt{n_1 p_+(1-p_+)}}\right) \longrightarrow \beta\ . \tag{15.5}$$

Thus equations (15.4) and (15.5) give

$$\alpha_{S_+} \longrightarrow \alpha \implies C_1(n_1) = n_1/2 + z_\alpha\sqrt{n_1/4}(1+o(1)) \tag{15.6}$$

$$\beta_{S_+} \longrightarrow \beta \implies C_1(n_1) = n_1 p_+ + z_\beta\sqrt{n_1 p_+(1-p_+)}(1+o(1)) \tag{15.7}$$

where $o(1) \to 0$ as $n_1 \to \infty$. Subtracting (15.6) from (15.7) gives

$$n_1(p_+ - 1/2) + \sqrt{n_1}(-z_\beta\sqrt{p_+(1-p_+)} - z_\alpha/2)(1+o(1))$$

and dividing by $\sqrt{n_1/4}$ we get

$$z_\alpha + z_\beta = (2p_+ - 1)\sqrt{n_1}(1+o(1))\ .$$

Table 15.2: Limiting Pitman efficiencies of S_+ relative to $\bar{X}$.

Density	$\psi(t)$	$e^P_{S_+,\bar{X}}$	
Uniform	$I[\lvert t\rvert < .5]$	$1/3$	0.333
Normal	$e^{-t^2/2}/\sqrt{2\pi}$	$2/\pi$	0.637
Logistic	$e^t/(1+e^t)^2$	$\pi^2/12$	0.822
Double Exp.	$e^{-\lvert t\rvert}/2$	2	2.000
Cauchy	$1/[\pi(1+t^2)]$	∞	∞

Similarly, for the $\bar{X}$ test we get

$$z_\alpha + z_\beta = \sqrt{n_2}(\mu_{n_2} - \mu_0)/\sigma$$

and equating $z_\alpha + z_\beta$ gives

$$\frac{n_2}{n_1} = \left(\frac{2p_+ - 1}{(\mu_{n_2} - \mu_0)/\sigma}\right)^2 .$$

Taking the limit as $n_1 \to \infty$ gives the limiting efficiency, due to Pitman, as

$$e^P_{s_+,\bar{X}} = \lim_{n_1\to\infty} \frac{n_2}{n_1} = \left(\lim_{n_1\to\infty} \frac{2\Phi((\mu_{n_2} - \mu_0)/\sigma) - 1}{(\mu_{n_2} - \mu_0)/\sigma}\right)^2 = \frac{2}{\pi} \doteq 0.637 .$$

Consider a distribution function $\Psi(t)$ with density $\psi(t)$ and median at $t = 0$ with finite variance σ^2. If the distribution $F(x) = \Psi(x - \mu)$, belongs to a location parameter family, then for testing $H: \ \mu = 0$ versus $A: \ \mu > 0$ we can similarly derive the limiting Pitman efficiency as

$$e^P_{s_+,\bar{X}} = 4\sigma^2\psi^2(0) \tag{15.8}$$

using the central limit theorem for S_+ and for $\bar{X}$. Table 15.1.2 gives values for several such distributions.

If we compare S_+ against the t test when σ^2 is unknown, the limits are the same as for comparing against $\bar{X}$.

15.1.5 Efficiency of the Median Point Estimator

If we calculate the variances of the sample median and sample mean for a normal $\mathcal{N}(\mu, \sigma^2)$ distribution we get the following table:

Table 15.3: Efficiency of $\tilde{X}$ relative to $\bar{X}$ for $\mathcal{N}(\mu, \sigma^2)$.

n	$\mathrm{Var}(\tilde{X})$	$\mathrm{Var}(\bar{X})$	$e_{\tilde{X},\bar{X}}$
1	1.0	1.0	1.000
3	0.449	0.333	0.742
5	0.287	0.200	0.696
7	0.210	0.143	0.681
9	0.1661	0.1111	0.668
11	0.1370	0.0909	0.664
13	0.1661	0.0769	0.658
15	0.1017	0.06667	0.656
17	0.09004	0.05882	0.653
19	0.08079	0.05263	0.651
∞	0	0	0.637

J.L. Hodges[1] suggests

$$\mathrm{Var}(\tilde{X}) \doteq \frac{2}{\pi}\left(1 - \frac{0.4324}{n}\right)$$

is a good approximation for the variance of the median for the $\mathcal{N}(0,1)$ distribution. $\mathrm{Var}(\bar{X}) = 1/n$ for $\mathcal{N}(0,1)$.

To get limiting efficiency, as $n \to \infty$, let $F(x) = \Psi(x-\mu)$, $\Psi(0) = 1/2$, and $d\Psi(t)/dt = \psi(t)$. We have, for $\tilde{X}$ =median$(X_1, X_2, \ldots, X_n)$,

$$\sqrt{n}(\tilde{X} - \mu) \xrightarrow{d} \mathcal{N}(0, [4\psi^2(0)]^{-1}) \text{ as } n \to \infty\ .$$

To see this, let $n = 2k+1$ so that the sample median$\tilde{X} = X_{(k+1)}$. Then

$$P_\mu[\sqrt{n}(X_{(k+1)} - \mu) \le u] = P_0[X_{(k+1)} \le u/\sqrt{n}]$$

where P_μ indicates the probability is calculated for $F(x) = \Psi(x-\mu)$. This in turn equals

$$P_0[\#(X_i \le u/\sqrt{n}) \ge k+1] = P_0[\#(X_i - u/\sqrt{n} \le 0) \ge k+1]$$

[1]Personal communication.

$$= P_{-u/\sqrt{n}}[\#(X_i \le 0) \ge k+1] = P_{-u/\sqrt{n}}[\#(X_i > 0) < k+1]$$

$$= P_{-u/\sqrt{n}}[S_+ < k{+}1] = P_{-u/\sqrt{n}}\left[(S_+ - np)/\sqrt{np(1-p)} < (k+1-np)/\sqrt{np(1-p)}\right]$$

where $p = P_{-u/\sqrt{n}}[X_i > 0] = 1 - H(u/\sqrt{n})$. Using

$$\frac{k+1-np}{\sqrt{np(1-p)}} = \left(\frac{(n+1)/2 - n(1-H(u/\sqrt{n}))}{\sqrt{n}/2}\right)\frac{\sqrt{n}/2}{\sqrt{np(1-p)}} \longrightarrow 2uh(0)$$

as $n \to \infty$ since $p \to 1/2$. The central limit theorem then gives

$$P_{-u/\sqrt{n}}\left[(S_+ - np)/\sqrt{np(1-p)} < (k+1-np)/\sqrt{np(1-p)}\right] \longrightarrow \Phi(2u\psi(0)) \ . \ \blacksquare$$

Using the central limit theorem for $\bar{X}$ we have for $E(X_i) = \mu_n$, $\mathrm{Var}(X_i) = \sigma^2$

$$\sqrt{n}(\bar{X} - \mu) \xrightarrow{d} \mathcal{N}(0, \sigma^2) \ .$$

If we define the limiting efficiency for these point estimators as the ratio of the variances of the limiting distributions then

$$e_{\tilde{X},\bar{X}} = \frac{\sigma^2}{[4\psi^2(0)]^{-1}} = 4\sigma^2\psi^2(0) \ .$$

This limit is the same as the limiting Pitman efficiency for the test of S_+ relative to $\bar{X}$ and gives $2/\pi \doteq 0.637$ for the $\mathcal{N}(\mu, \sigma^2)$ distribution.

15.2 The Wilcoxon Signed Rank Test

We note that the efficiency of the sign test is not particularly high when compared to the $\bar{X}$ or t test for $\mathcal{N}(\mu, \sigma^2)$ alternatives. If we are willing to also assume that under the null hypothesis the distribution is symmetric about the median then there is a nonparametric test with much better efficiency.

Let the sample $X_1, X_2, \ldots, X_n$ be independent with continuous c.d.f. $F(x)$. For the hypothesis

$$H_1: \ F(x) \text{ is symmetric about the median } \mu = 0 \text{ versus } A_1: \ \mu > 0$$

the Wilcoxon[2] signed rank statistic is

$$W_+ = \sum_{k=1}^{n} k z_k \text{ where } z_k = \begin{cases} 1 & \text{if } X_{[k]} > 0 \\ 0 & \text{if } X_{[k]} < 0 \end{cases}$$

[2]Wilcoxon, Frank (1945). Individual comparisons by ranking methods. *Biometrics* **1**, 80-83

and $X_{[k]}$ is the k th largest in magnitude of the sample:

$$|X_{[1]}| < |X_{[2]}| < \cdots < |X_{[n]}| \ .$$

Thus W_+ is the sum of the magnitude ranks for those observations that are positive. We reject H_1 in favor of A_1 if $W_+ \geq C_1$ where $P_H[W_+ \geq C_1] = \alpha$

We note that if $X_i = X_i' - X_i''$ where (X_i', X_i'') are both independent with the same distribution under H then X_i have a symmetric null distribution in this paired comparisom case.

15.2.1 Null Distribution of W_+

If F is symmetric about $\mu = 0$ then

$$P_H[Z_1 = z_1, Z_2 = z_2, \ldots, Z_n = z_n] = \frac{1}{2^n} \text{ where } z_k \in \{0, 1\} \ .$$

Then

$$P_H[W_+ = w] = \frac{a(w, n)}{2^n}$$

where $a(w, n)$ is the number of vectors $(z_1, z_2, \ldots, z_n)$ for which $\sum_{k=1}^n k z_k = w$.

We can calculate $a(w, n)$ from the recursion equation

$$a(w, n) = a(w, n-1) + a(w-n, n-1)$$

with $a(-k, n) = 0 = a(n(n+1)/2+k, n)$ for integer $k \geq 1$ and $a(0, 1) = 1 = a(1, 1)$. This equation is shown as follows by adding numbers for $z_n = 1$ and $z_n = 0$:

$$a(w, n) = \#\{(z_1, z_2, \ldots, z_n) : \sum_{k=1}^n k z_k = w\}$$

$$= \#\{(z_1, z_2, \ldots, z_{n-1}, 0) : \sum_{k=1}^{n-1} k z_k = w\}$$

$$+\#\{(z_1, z_2, \ldots, z_{n-1}, 1) : \sum_{k=1}^{n-1} k z_k = w - n\}$$

$$= a(w, n-1) + a(w-n, n-1) \ . \ \blacksquare$$

Table 15.4: $2^n P[W_+ = w]$ for $n = 1(1)12$, $w = 0(1)15$.

w	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
n=1	1	1														
2	1	1	1	1												
3	1	1	1	2	1	1	1									
4	1	1	1	2	2	2	2	2	1	1	1					
5	1	1	1	2	2	3	3	3	3	3	3	2	2	1	1	1
6	1	1	1	2	2	3	4	4	4	5	5	5	5	4	4	4
7	1	1	1	2	2	3	4	5	5	6	7	7	8	8	8	8
8	1	1	1	2	2	3	4	5	6	7	8	9	10	11	12	13
9	1	1	1	2	2	3	4	5	6	8	9	10	12	13	15	17
10	1	1	1	2	2	3	4	5	6	8	10	11	13	15	17	20
11	1	1	1	2	2	3	4	5	6	8	10	12	14	16	19	22
12	1	1	1	2	2	3	4	5	6	8	10	12	15	17	20	24

If we define $W_- = \sum_{k=1}^n k(1 - z_k)$ then the distribution of W_- is the same as that of W_+ under the hypothesis of symmetry about $\mu = 0$. Thus since

$$W_+ + W_- = \sum_{k=1}^n k = \frac{n(n+1)}{2}$$

we have $a(w, n) = a(n(n+1)/2 - w, n)$ and the distribution is symmetric about $n(n+1)/4$. Table 15.4 gives the distribution of $2^n P[W_+ = w]$ for $n \leq 12$.

15.2.2 Zeros and Ties

When zeros and ties are present, Prat(1959)[3] recommends using the zeros in ranking the magnitudes and using average ranks for the magnitude ties. If $0 < z_1 < z_2 < \cdots < z_K$ are the distinct magnitudes then the counts for the observations $X_1, X_2, \ldots, X_n$ can be set up in a table:

[3]Prat, J.W. (1959) Remarks on zeros and ties in the Wilcoxon signed rank procedures. *Journal of the American Statistical Association* **54**, 655-667.

Magnitudes	0	z_1	z_2	$\cdots$	z_K
$\#(X_i > 0)$		u_1	u_2	$\cdots$	u_K
$\#(X_i < 0)$		v_1	v_2	$\cdot$	v_K
Total	t_0	t_1	t_2	$\cdots$	t_K

Then with $a_i(\boldsymbol{t})$ the average ranks for the observations with tied magnitude z_i, the statistic

$$W_+ = \sum_{i=1}^{K} u_i a_i(\boldsymbol{t}), \quad W_- = \sum_{i=1}^{K} v_i a_i(\boldsymbol{t})$$

where $\boldsymbol{t} = (t_0, t_1, \ldots, t_K)$ and $a_i(\boldsymbol{t}) = t_0 + t_1 + \cdots + t_{i-1} + (t_i + 1)/2$.

Klotz (1992)[4] gave an algorithm for calculating the exact distribution and later improved it using linked lists[5]

For large samples, a normal approximation can be used with

$$Z = \frac{W_+ - E(W_+|\boldsymbol{t})}{\sqrt{Var(W_+|\boldsymbol{t})}}$$

where

$$E(W_+|(t_0, t_1, \ldots, t_K)) = \frac{n(n+1) - t_0(t_0+1)}{2}$$

and

$$Var(W_+|(t_0, t_1, \ldots, t_K)) =$$

$$\frac{n(n+1)(2n+1) - t_0(t_0+1)(2t_0+1)}{24} - \frac{\sum_{i=1}^{K} t_i(t_i-1)(t_i+1)}{48}.$$

A subroutine **Wilcox.h** uses a linked list to calculate the Wilcoxon signed rank distribution with provision for ties in appendix J. Th program **sRank.cpp** in appendix K uses the subroutine to calculate P-values for the test with input a set of numbers in a file. If the sample size $n \leq 200$ exact P-valuses are given in addition to P-values from the normal approximation. For example if the data in file *sRank.data* is $(X_1, X_2, \ldots, X_{15}) =$

$$(5.0,\ -4.0,\ 0,\ 3.0,\ 2.0,\ -5.0,\ -1.0,\ -3.0,\ 4.0,\ 0,\ -4.0,\ 2.0,\ -3.0,\ -3.0,\ -2.0)$$

with the table of counts

[4]Klotz, J.H.(1992) Exact computation of the Wilcoxon signed rank distribution with zeros and ties. *Computing Science and Statistics (Interface 90). Proceedings of the 22nd Symposium on the Interface.* Springer-Verlag. N.Y. 397-400.

[5]Klotz, Jerome (1998) A linked list for the Wilcoxon signed rank test. *Nonparametric Statistics* **9** 88-93.

Magnitudes	0	1.0	2.0	3.0	4.0	5.0
$\#(X_i > 0)$		0	2	1	1	1
$\#(X_i < 0)$		1	1	3	2	1
Total	2	1	3	4	3	2

and average ranks $\boldsymbol{a} = (3, 5, 8.5, 12, 14.5)$, then compiling the program sRank.cpp
g++ -o sRank sRank.cpp
and then executing it with
sRank sRank.data
gives the following output:

```
Wilcoxon signed rank test for data in Test.data .

Average magnitude ranks are used with zeros and ties.
Zeros are used to form average magnitude ranks with
W+ the sum of these ranks for positive observations.

W+=45 for sample size n= 15.

Lower tail P-value P(W+<=45 |5,t)= 0.22998046875

Upper tail P-value P(W+>=45 |5,t)= 0.78173828125

Two sided P-value= 0.4599609375 .

Normal approximation with zeros and ties correction:

approximate lower tail P-value 0.2203

approximate upper tail P-value 0.7797

approximate two tailed P-value 0.4405.

E(W+)=    58.5 , Var(W+)= 306.375, z= -0.77127 .
```

The limiting normal distribution of W_+ under the hypothesis as $n \to \infty$ can be established using the Liapounov form of the central limit theorem (see Theorem 9.14).

15.2.3 Wilcoxon Point Estimate for the Center of Symmetry

Let $X_1, X_2, \ldots, X_n$ be independent with c.d.f $F(x) = \Psi(x - \mu)$ where $\Psi(t)$ is continuous and symmetric about $t = 0$ ($\Psi(-t) = 1 - \Psi(t)$). The statistic

$$W_+ = \sum_{1 \le i \le k \le n} \sum I[\frac{X_i + X_j}{2} > 0]$$

since if we define $X_{[1]}, X_{[2]}, \ldots, X_{[n]}$ to be the observations sorted by magnitude, $|X_{[1]}| < |X_{[2]}| < \cdots < |X_{[n]}|$, then

$$\sum_{1 \le i \le k \le n} \sum I[\frac{X_i + X_j}{2} > 0] = \sum_{k=1}^{n} \sum_{r=1}^{k} I[\frac{X_{[r]} + X_{[k]}}{2} > 0]$$

$$= \sum_{k=1}^{n} kI[X_{[k]} > 0] = \sum_{k=1}^{n} kz_k = W_+$$

where $z_k = 1$ if $X_{[k]} > 0$ and 0 otherwise. Recall the values $(X_i + X_j)/2$ for $i \le j$ are Walsh sums. Thus W_+ is the number of positive Walsh sums out of the total $n(n+1)/2$.

For testing $H: \ \mu = \mu_0$ versus $A: \ \mu \ne \mu_0$ consider the acceptance region using $W_+(\mu_0)$ which is the Wilcoxon signed rank test statistic calculated for the observations $X_i - \mu_0$ for $i = 1, 2, \ldots, n$. The $1 - \alpha$ probability region is

$$\mathcal{A}(\mu_0) = \{(X_1, X_2, \ldots, X_n): \ C < W_+(\mu_0) < n(n+1)/2 - C\}$$

where the critical value C satisfies

$$P[W_+ \le C] = \frac{\alpha}{2} \ .$$

The associated confidence set is

$$\mathcal{S}(X_1, X_2, \ldots, X_n) = \{\mu: \ C < W_+(\mu) < (n(n+1)/2) - C\} \ .$$

Using

$$W_+(\mu) = \sum_{1 \le i \le k \le n} \sum I[\frac{X_i + X_j}{2} > \mu]$$

and the event

$$[C < W_+(\mu)] = [\mu < w_{(n(n+1)/2-C)}]$$

where $w_{(1)} < w_{(2)} < \cdots < w_{(n(n+1)/2)}$ are the sorted Walsh sums. We have $W_+(\mu) < C$ implies at least $C+1$ of the ordered Walsh sums exceed μ namely the $C+1$ Walsh sums $w_{(n(n+1)/2-C)}, w_{(n(n+1)/2-C+1)}, \ldots, w_{(n(n+1)/2)}$. Thus

$$\mathcal{S}(X_1, X_2, \ldots, X_n) = \{\mu : \ w_{(C+1)} \leq \mu < w_{(n(n+1)/2-C)}\} \ .$$

For an example, consider the 12 data values

4.9	6.0	6.9	17.6	4.5	12.3	5.7	5.3	9.6	13.5	15.7	1.7

The $12 \times 13/2 = 78$ sorted Walsh sums are

1.70	3.10	3.30	3.50	3.70	3.85	4.30	4.50	4.70
4.90	4.90	5.10	5.10	**5.25**	5.30	5.30	5.45	5.50
5.65	5.65	5.70	5.70	5.85	5.90	6.00	6.10	6.30
6.45	6.90	7.00	7.05	7.25	7.45	7.60	7.65	7.80
8.25	8.40	<u>8.60</u>	<u>8.70</u>	8.80	9.00	9.00	9.15	9.20
9.40	9.60	9.60	9.60	9.65	9.75	10.10	10.20	10.30
11.65	**11.80**	12.25	12.30	12.65	12.90	13.50	13.60	14.00
14.60	14.95	15.55	15.70	16.65	17.60			

To construct a confidence interval with confidence coefficient just excceding 0.95 we have from table 15.4, $P_H[W_+ \leq 13|n = 12] = 87/2^{12} \doteq 0.0212402$ and the exact confidence coefficient is $1 - \alpha = 1 - 174/2^{12} \doteq 0.9575196$. The value of the confidence interval is

$$[w_{(14)}, w_{(65)}) = [5, 25, 11, 80) \ .$$

The point estimator for μ is the median of the sorted Walsh sums. For the example it is (8.60+8.70)/2=8.65 .

15.2.4 Efficiency of W_+

The limiting Pitman efficiency for "near-by" location alternatives ($F(x) = \Psi(x - \mu_n)$) where $\mu_n = O(1/\sqrt{n})$) relative to the t-test is given by

$$e^P_{W_+,t} = 12\sigma^2 \left[\int_{-\infty}^{\infty} \psi^2(t)dt\right]^2 \tag{15.9}$$

Table 15.5: Limiting Pitman efficiencies of W_+ relative to $\bar{X}$ or t.

Density	$\psi(t)$	$e^P_{W_+,t}$	
Parabolic	$3(5-t^2)I[t^2<5]/(20\sqrt{5})$	$108/125$	0.864
Normal	$e^{-t^2/2}/\sqrt{2\pi}$	$3/\pi$	0.955
Uniform	$I[\|t\|<.5]$	1	1.000
Logistic	$e^t/(1+e^t)^2$	$\pi^2/9$	1.097
Double Exp.	$e^{-\|t\|}/2$	$3/2$	1.500
Cauchy	$1/[\pi(1+t^2)]$	∞	∞

where $\psi(t)$ is the density of $\Psi(t)$ and σ^2 is the variance for Ψ. Table (15.5) gives values for various densities.

Hodges and Lehmann (1956)[6], using a calculus of variations argument, show that $e^P_{W_+,t}(H) \geq 0.864$ for all distributions. This lower bound is attained for the patabolic density. Klotz (1963)[7], using a computation scheme of Hodges, showed that small sample efficiency for normal shift alternatives is close to the limiting Pitman efficiency value.

The limiting efficiency of the Walsh sum median point estimator relative to $\bar{X}$, by an argument similar to that for the sign test and median, is is also given by equation (15.9) where σ^2/n is the variance of $\bar{X}$.

15.3 The Two Sample Median Test

Let $X_1, X_2, \ldots, X_m$ be independent with c.d.f. $F(x)$ and $Y_1, Y_2, \ldots, Y_n$ be independent with c.d.f. $G(x)$. For testing the hypothesis

$$H: \ G = F \text{ versus } A: \ G > F \tag{15.10}$$

[6]Hodges, J.L. and E.L. Lehmann (1956) Efficiencies of some nonparametric competitors of the t-test. *Annals of Mathematical Statistics* **27**, 324-335.

[7]Klotz, J.H. (1963) Small sample power and efficiency for the one sample Wilcoxon and normal scores tests. *Annals of Mathematical Statistics* **34** 624-632.

Mood and Brown (1950)[8] proposed the two sample median test. Let $\tilde{Z}$ be the median of the combined sample $X_1, X_2, \ldots, X_m, Y_1, Y_2, \ldots, Y_n$ and define

$$B = \sum_{i=1}^{m} I[X_i > \tilde{Z}]$$

the number of X_i that exceed $\tilde{Z}$. If B is large, we reject H in favor of A (a shift of the X sample to the right of the Y sample).

The null distribution of B is the hypergeometric(N, m, a)

$$P_H[B = b] = \binom{m}{b}\binom{n}{a-b} \Big/ \binom{N}{a} \text{ for } b = L, L+1, \ldots, U$$

where $N = m + n$, $L = \max(0, m + a - N)$, $U = \min(m, a)$, and

$$a = \sum_{i=1}^{m} I[X_i > \tilde{Z}] + \sum_{j=1}^{n} I[Y_j > \tilde{Z}]$$

is the number of observations in the pooled sample greater than $\tilde{Z}$.
If N is even and there are no ties, then $a = N/2$.

15.3.1 Confidence Interval for a Difference in Location Parameters

If $F(x) = \Psi(x - \mu)$ and $G(x) = \Psi(x - \eta)$, with $\Delta = \mu - \eta$, then for testing $H: \ \Delta = \Delta_0$ we can use the statistic

$$B(\Delta_0) = \sum_{i=1}^{m} I[X_i - \Delta_0 > \tilde{Z}(\Delta_0)]$$

where $\tilde{Z}(\Delta_0)$ is the median for the combined sample

$$X_1 - \Delta_0, X_2 - \Delta_0, \ldots, X_m - \Delta_0, Y_1, Y_2, \ldots, Y_n \ .$$

The acceptance region with probability $1 - \alpha$ for the approximately equal tailed two sided test is

$$\mathcal{A}(\Delta_0) = \{(X_1, X_2, \ldots, X_m, Y_1, Y_2, \ldots, Y_n) : C_1 < B(\Delta_0) < C_2\}$$

[8]Mood, A.M. (1950) *Introduction to the Theory of Statistics.* McGraw-Hill, New York.

where

$$P_H(B \le C_1) = \alpha_1, \quad P_H(B \ge C_2) = \alpha_2, \quad \alpha = \alpha_1 + \alpha_2$$

and $\alpha_1, \alpha_2 \le \alpha^*/2$ are both as close to $\alpha^*/2$ as possible where $1 - \alpha^*$ is the nominal confidence coefficient. The associated confidence set for Δ is

$$\mathcal{S}(X_1, X_2, \ldots, X_m, Y_1, Y_2, \ldots, Y_n) = \{\Delta : \ C_1 < B(\Delta) < C_2\} \ .$$

Using the relation

$$[B(\Delta) \ge b] = [Y_{(n-(a-b))} < X_{(m-b+1)} - \Delta] = [\Delta < X_{(m-b+1)} - Y_{(n-(a-b))}]$$

since at least b of the $X_i - \Delta$, namely the sorted values

$$X_{(m-b+1)} - \Delta, X_{(m-b+2)} - \Delta, \ldots, X_{(m)} - \Delta,$$

must be greater than the observations that contain the median $\tilde{Z}(\Delta)$ which include at least

$$X_{(1)} - \Delta, X_{(2)} - \Delta, \ldots, X_{(m-b)} - \Delta, Y_{(1)}, Y_{2)}, \ldots, Y_{(n-(a-b))} \ .$$

Note $(m - b) + (n - (a - b)) = N - a$ which is the number of observations less than or equal $\tilde{Z}$. Thus

$$\begin{aligned}
&[C_1 < B(\Delta) < C_2] = [B(\Delta) \ge C_2]^c \cap [B(\Delta) \ge C_1 + 1] \\
&= [\Delta < X_{(m-C_2+1)} - Y_{(n-a+C_2)}]^c \cap [\Delta < X_{(m-C_1)} - Y_{(n-a+C_1+1)}] \\
&= [X_{(m-C_2+1)} - Y_{(n-a+C_2)} \le \Delta < X_{(m-C_1)} - Y_{(n-a+C_1+1)}] \\
&= [X_{(m-C_2+1)} - Y_{(n-a+C_2)}, \ \ X_{(m-C_1)} - Y_{(n-a+C_1+1)}) \ .
\end{aligned}$$

15.3.2 Efficiency of the Mood and Brown Test

For $F(x) = \Psi(x - \mu)$ and $G(x) = \Psi(x - \eta)$ where $\Psi(x)$ has density $\psi(x)$ then using asymptotic theory for "near-by" altermatives $\Delta = \mu - \eta = \Delta_N = O(1/\sqrt{N})$ we obtain the limiting Pitman efficiency of B relative to the two sample t test for these location parameter distributions as $N \to \infty$, $\lambda_N = m/N \to \lambda$ where $0 < \lambda < 1$ is

$$4\sigma^2\psi^2(0)$$

where σ^2 is the variance of the distribution $\Psi(x)$. Table 15.6 gives values for various densities as in table 15.2 for the sign test.

Table 15.6: Limiting Pitman efficiencies of B relative to t.

Density	$\psi(t)$	$e^P_{B,t}$	
Uniform	$I[\|t\| < .5]$	$1/3$	0.333
Normal	$e^{-t^2/2}/\sqrt{2\pi}$	$2/\pi$	0.637
Logistic	$e^t/(1+e^t)^2$	$\pi^2/12$	0.822
Double Exp.	$e^{-\|t\|}/2$	2	2.000
Exponential	$e^{-t}I[t > 0]$	4	4.000
Cauchy	$1/[\pi(1+t^2)]$	∞	∞

15.4 The Two Sample Wilcoxon Rank Test

Another test for the hypothesis (15.10) is that of the Wilcoxon two sample rank sum test [9]. For the two samples $(X_1, X_2, \ldots, X_m)$ and $(Y_1, Y_2, \ldots, Y_n)$ from continuous distributions (so there are no ties), let $R(X_i)$ be the rank in the pooled sample of $N = m + n$ observations. We reject H in favor of A if

$$W_X = \sum_{i=1}^{m} R(X_i)$$

is large. An alternate equivalent statistic due to Mann and Whitney[10] is

$$U_{YX} = \sum_{i=1}^{m}\sum_{j=1}^{n} I[Y_j < X_i] = W_X - \frac{m(m+1)}{2}\,.$$

To show this we have

$$U_{YX} = R(X_{(1)}) - 1 + R(X_{(2)}) - 2 + \cdots + R(X_{(m)}) - m = W_X - m(m+1)/2\,.$$

15.4.1 Null Distribution of U_{YX}

The null distribution of U_{YX} is the same as that for U_{XY}. To prove this let W_X^*, W_Y^* be the values of the statistics where we rank the observations in

[9] Wilcoxon, Frank (1945). Individual comparisons by ranking methods. *Biometrics* **1**, 80-83

[10] Mann, H. B. and Whitney, D.R. (1947). On a test of whether one of two random variables is stochastically larger than another. *Annals of Mathematical Statisticsis* **18**, 50-60.

reverse order (from largest to smallest). Then

$$W_X^* = \sum_{i=1}^{m} R^*(X_i) = \sum_{i=1}^{m}(N+1-R(X_i)) = m(N+1) - W_X$$

where $R^*(X_i)$ is the rank in decreasing order of X_i and $R(X_i)$ is the rank in increasing order. Thus

$$W_X - m(N+1)/2 = m(N+1)/2 - W_X^*$$

Since the joint null distribution of the ranks $R^*(X_i)$ is the same as that for $R(X_i)$, namely $1/\binom{N}{m}$, we have

$$P_H[W_X - m(N+1)/2 = w] = P_H[m(N+1)/2 - W_X = w] \ . \qquad (15.11)$$

Now using $W_X + W_Y = N(N+1)/2$ we have $W_X - m(N+1)/2 = m(N+1)/2 - W_Y$ so from (15.11) we get

$$P_H(U_{YX} = u] = P_H[(W_X - m(N+1)/2) + mn/2 = u]$$

$$= P_H[(m(N+1)/2 - W_X) + mn/2 = u] = P[W_Y - n(N+1)/2 + mn/2 = u]$$
$$= P_H[W_Y - n(n+1)/2 = u] = P_H[U_{XY} = u] \ .$$

Since $U_{YX} = mn - U_{XY}$ the distribution of U_{YX} is symmerric about $mn/2$ for the case of no ties.

Let $U = U_{XY}$ or U_{YX}. If we define

$$P_H[U = u] = \frac{a(u|N,m)}{\binom{N}{m}},$$

we have the recursion equation

$$a(u|N,n) = a(u|N-1,m) + a(u-n|N-1,m-1)$$

since the largest value in the pooled sample is either a Y value or an X value for $U = U_{YX}$. If $A(u|N,m) = \sum_{k=0}^{u} a(k|N,m)$ is the cumulative, then also

$$A(u|N,n) = A(u|N-1,m) + A(u-n|N-1,m-1)$$

with side conditions

$$A(u|N,n) = 0 \text{ for } u < 0, \text{ and } A(u|N,n) = \binom{N}{m} \text{ for } u \geq mn.$$

A variety of tables exist. In particular Milton (1964)[11] gives critical values. Fix and Hodges (1955)[12] use this recursion formula and partition theory to extend the calculation of exact probabilities.

15.4.2 Distribution of U_{YX} in the Presence of Ties

Consider the discrete case where the observations can only take on the values $z_1 < z_2 < \cdots < z_K$. Let

$$P[X_i = z_k] = p_k \text{ and } P[Y_j = z_k] = r_k$$

where $\sum_{k=1}^K p_k = 1 = \sum_{k=1}^K r_k$. The hypothesis is then $H: \ p_k = r_k$ and the distributions under H are

$$P_H(\mathbf{X} = \mathbf{x}) = p_1^{u_1} p_2^{u_2} \cdots p_K^{u_k}, \quad P_H(\mathbf{Y} = \mathbf{y}) = p_1^{v_1} p_2^{v_2} \cdots p_K^{v_k}$$

and for $\mathbf{X} = (X_1, X_2, \ldots, X_m)$, $\mathbf{x} = (x_1, x_2, \ldots, x_m)$ $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_n)$, $\mathbf{y} = (y_1, y_2, \ldots, y_m)$

$$P_H(\mathbf{X} = \mathbf{x}, \mathbf{Y} = \mathbf{y}) = p_1^{t_1} p_2^{t_2} \cdots p_K^{t_k}$$

where the counts

$$u_k = \sum_{i=1}^m I[x_i = z_k], \quad v_k = \sum_{j=1}^n I[y_j = z_k], \text{ and } t_k = u_k + v_k \ .$$

Thus $T_k = U_k + V_k = \sum_{i=1}^m I[X_i = z_k] + \sum_{j=1}^n I[Y_j = z_k]$ for $k = 1, 2, \ldots, K$ is sufficient for $\mathbf{p} = (p_1, p_2, \ldots, p_K)$ under H. We can construct a distribution free test by conditioning on $\mathbf{T} = (T_1, T_2, \ldots, T_K)$. We have

$$P_H(\mathbf{U} = \mathbf{u} | \mathbf{T} = \mathbf{t}) = \left(m! \prod_{k=1}^K \frac{p_k^{u_k}}{u_k!} \right) \left(n! \prod_{k=1}^K \frac{p_k^{v_k}}{v_k!} \right) / \left(N! \prod_{k=1}^K \frac{p_k^{t_k}}{t_k!} \right) = \prod_{k=1}^K \binom{t_k}{u_k} / \binom{N}{m} \ .$$

[11] Milton, R.(1964) An extended table of critical values for the Mann-Whitney (Wilcoxon) two sample statistic. *Journal of the American Statistical Association* **59**,925-934.

[12] Fix, E. and Hodges, J.L.,Jr.(1955). Significance probabilities of the Wilcoxon test. *Annals of Mathematical Statistics* **26**, 301-312.

Putter (1955)[13] recommends using average ranks $R^*(X_i)$ for the Wilcoxon rank sum statistic

$$W_X^* = \sum_{i=1}^{m} R^*(X_i) = \sum_{k=1}^{K} u_k r_k^*$$

where the k-th largest average rank is

$$r_k^* = t_1 + t_2 + \cdots + t_{k-1} + \frac{t_k + 1}{2} \text{ for } k = 2, 3, \ldots, K$$

and $r_1^* = (t_1 + 1)/2$. The equivalent Mann Whitney form is

$$U_{YX} = (U_1, U_2, \ldots, U_K) \begin{pmatrix} 1/2 & 0 & \cdots & 0 \\ 1 & 1/2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1/2 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ V_K \end{pmatrix} = \mathbf{UQV^T}$$

which satisfies

$$U_{YX} = \sum_{i=1}^{m} \sum_{j=1}^{n} \left(I[Y_j < X_i] + \frac{1}{2} I[Y_j = X_i] \right) = W_X^* - \frac{m(m+1)}{2} \ .$$

The exact distribution is given by

$$P_H(U_{YX} \leq x | \mathbf{T} = \mathbf{t}] = \sum_{\mathbf{u} \in \mathcal{R}(x)} \left\{ \prod_{k=1}^{K} \binom{t_k}{u_k} \Big/ \binom{N}{m} \right\}$$

where

$$\mathcal{R}(x) = \{\mathbf{u} : \ \mathbf{uQ}(\mathbf{t} - \mathbf{u})^{\mathbf{T}} \leq x\} \ .$$

Klotz (1966)[14] developed an early program using this scheme by generating all possible vectors $(u_1, u_2, \ldots, u_K)$ with $\sum_{k=1}^{K} u_k = m$ and $0 \leq u_k \leq t_k$ for $k = 1, 2, \ldots, K$. Mehta et. al.(1984)[15] improved this scheme by eliminating some unnecessary vectors in the generation. Cheung and Klotz (1997)[16]

[13]Putter, J.(1955). The treatment of ties in some nonparametric tests. *Annals of Mathematical Statistics* **26**, 368-386.

[14]Klotz, J.H. (1966) The Wilcoxon, ties, and the computer. *Journal of the American Statistical Association* **61**, 772-787.

[15]Mehta, C.R., Patel, N.R. and Tsiatis, A.A. (1984). Exact significance testing to establish treatment equivalence with ordered categorical data. *Biometrics* **40**, 819-825.

[16]Cheung, Y.K. and Klotz, J.H. (1997). The Mann Whitney Wilcoxon distribution using linked lists. *Statistica Sinica* **7**, 805-813.

furthur improved the distribution calculation by using a linked list. The subroutine **MannW.h** in appendix L calculates the distribution for given values of $\mathbf{t}$ and m. The program **RankSum.cpp** in appendix M gives exact P-values for $N \leq 100$ and approximate P-values using the normal approximation for

$$Z = \frac{U_{YX} - E_H(U_{YX}|\mathbf{t})}{\sqrt{Var_H(U_{YX}|\mathbf{t})}}$$

where

$$E_H(U_{YX}|\mathbf{t}) = \frac{mn}{2}, \quad Var_H(U_{YX}|\mathbf{t}) = \frac{mn(N+1)}{12}\left(1 - \frac{\gamma}{N^3 - N}\right),$$

and $\gamma = \sum_{k=1}^{K}(t_k^3 - t_k)$ is the correction for ties. Note $\gamma = 0$ if there are no ties ($t_i = 1$ for all $i = 1, 2, \ldots, K = N$).

For example if the file **dataX** contains the values

18 14.5 13.5 12.5 23 24 21 17 18.5 9.5 14

and the file **dataY** contains the values

27 34 20.5 29.5 20 28 20 26.5 22 24.5 34 35.5 19

then compiling the program using the gnu C++ compiler with **g++ -o RankSum RankSum.cpp** and executing the program with **RankSum dataX dataY** we obtain the following output:

```
P-values for the Wilcoxon Mann Whitney two sample rank sum test for the
X sample data in file ‘dataX’ and the Y sample data in file ‘dataY’.

Using the exact distribution:
UYX = 14, m= 11, n= 13
Lower tail P-value is P(UYX<=14|m, t)= 0.000184284
Upper tail P-value is P(UYX>=14|m, t)= 0.999839
For the two sided test which rejects for |UYX-E(UYX)|>=C
the P-value is P(UYX<=14|m,t)+P(UYX>=129|m,t)= 0.000371773 .

Using the normal approximation with
UYX = 14, m= 11, n= 13
E(UYX)=71.5, Var(UYX)=297.658, sigma(UYX)=17.2528
Z=(UYX-E(UYX))/sigma(UYX)=-3.3328
```

```
Approximate lower tail P-value is 0.000429882
Approximate upper tail P-value is 0.99957
Approximate P-value for the two sided test is 0.000859765
for ties
t=(1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 1).
K= 22, sum(t[i]^3-t[i])= 12 .
```

15.4.3 Confidence Intervals for a Location Difference

If $F(x) = \Psi(x - \mu)$ and $G(x) = \Psi(x - \eta)$, are continuous with $\Delta = \mu - \eta$, then for testing $H: \ \Delta = \Delta_0$ we can use the statistic

$$U_{YX}(\Delta_0) = \#\{X_i - \Delta_0 < Y_j : \text{ for } i = 1, 2, \ldots, m; j = 1, 2, \ldots, n\} \ .$$

If the acceptance region for the two sided test is

$$\mathcal{A}(\Delta_0) = \{(X_1, X_2, \ldots, X_m, Y_1, Y_2, \ldots, Y_n) : \ C_1 < U_{YX}(\Delta_0) < C_2\}$$

then the corresponding confidence interval for Δ is

$$\mathcal{S}(X_1, X_2, \ldots, X_m, Y_1, Y_2, \ldots, Y_n) = \{\Delta : \ C_1 < U_{YX}(\Delta) < C_2\} \ .$$

Let $W_{(1)} < W_{(2)} < \cdots < W_{(mn)}$ be the sorted values of $X_i - Y_j$ for $i = 1, 2, \ldots, m$ and $j = 1, 2, \ldots, n$. Then we have the relation

$$[U_{YX}(\Delta) \geq k] = [W_{(mn-k+1)} > \Delta]$$

since if at least k of the differences $X_i - Y_j$ are greater than Δ, they are $W_{(mn-k+1)}, W_{(mn-k+2)}, \ldots, W_{(mn)}$. Thus

$$\mathcal{S}(X_1, X_2, \ldots, X_m, Y_1, Y_2, \ldots, Y_n) = \{\Delta : \ W_{(mn-C_2+1)} \leq \Delta < W_{(mn-C_1)}\}$$

If we use an equal tail test, with C_1 chosen such that

$$\frac{\alpha}{2} = P_H(U_{YX} \leq C_1)$$

then using the symmetry for the distribution without ties, $C_2 = mn - C_1$ and the confidence interval for Δ is then $[W_{(C_1+1)}, W_{(mn-C_1)})$. We count in $C_1 + 1$ values from both ends of $W_{(1)} < W_{(2)} < \cdots < W_{(mn)}$.

If $\Psi(x)$ is not continuous then the confidence interval that includes both endpoints

$$\{\Delta : \ W^*_{(mn-C_2+1)} \leq \Delta \leq W^*_{(mn-C_1)}\}$$

where $W^*_{(1)} \leq W^*_{(2)} \leq \cdots \leq W^*_{(mn)}$ are sorted values of $Y_j - X_i$, has probability of covering Δ at least $1-\alpha$. Here $\alpha = \alpha_1 + \alpha_2$ and

$$\alpha_1 = P_H(U_{YX} \leq C_1), \quad \alpha_2 = P_H(U_{YX} \geq C_2)$$

is computed using the null distribution without ties. For a proof, see Randales and Wolfe (1979)[17] pages 182,183.

For example, if the X sample values are

2.7 3.2 4.5 7.6 8.1

and the Y sample values are

0.8 1.6 1.9 2.2 3.7 4.3 8.0

then the sarted differences are

-5.3	-4.8	-3.5	-1.4	-1.0	-0.9	**-0.5**
-0.4	0.1	0.2	0.5	0.8	0.8	1.0
1.1	1.3	1.6	**1.9**	2.3	2.4	2.6
2.9	3.3	3.7	3.8	3.9	4.4	5.4
5.7	5.9	6.0	6.2	6.5	6.8	7.3

.

If we use $C_1 = 6$ and $C_2 = 29$ then $P(U_{YX} \leq 6) = P(U_{YX} \geq 29) = 29/792 \doteq 0.0366162$ and $P(6 < U_{YX} < 29) = 734/792 \doteq 0.9267677$. Thus counting in 7 from each end, the value of the confidence interval with probability at least 0.9267677 is $[W_{(7)}, W_{(29)}] = [-0.5, 5.7]$.

Hodges and Lehmann (1963)[18] recommend the point estimator for Δ given by

$$\hat{\Delta} = \text{median}\{Y_j - X_i : \ i = 1, 2, \ldots, m; j = 1, 2, \ldots, n\} \ .$$

In the example above, $\hat{\Delta} = 1.9$.

[17] Randals, R.H. and Wolfe, D.A. (1979). *Introduction to the Theory of Nonparametric Statistics.* John Wiley & Sons, New York.

[18] Hodges, J.L.,Jr. and Lehmann, E.L. (1962). Estimates of location based on rank tests. *Annals of Mathematical Statistics* **34**, 598-611.

15.4.4 Efficiency of the Two Sample Wilcoxon

Noether (1955)[19] presented a theoren for comparing the efficiency of two tests for a sequence of alternative distributions converging to the null hypothesis (so called *near by* alternatives). The theorem established the relative efficiency under several assumptions, including the common limiting distribution such as the normal, as a ratio of the squares of the efficacies of the two tests.

For the two sample Wilcoxon Mann Whitney test, the Hoeffding (1948)[20] paper on U statistics proved the asymptotic normality of U_{YX}. It can also be shown for W_X using the theory of Chernoff and Savage (1958)[21].

For $F(x) = \Psi(x - \Delta_N)$, $G(x) = \Psi(x)$ with $\Delta_N = O(1/\sqrt{N})$, and $\lambda_N = m/N \to \lambda$ where $0 < \lambda < 1$ as $N \to \infty$, the efficacy for U_{YX} is

$$\mathcal{E}_{U_{YX}} = \lim_{N\to\infty} \frac{dE_\Delta(U_{YX})/d\Delta|_{\Delta=0}}{\sqrt{NVar_0(U_{YX})}} = \sqrt{12\lambda(1-\lambda)} \int_{-\infty}^{\infty} \psi^2(x)dx \ .$$

Similarly, for the two sample t test the efficacy is

$$\mathcal{E}_t = \sqrt{\lambda(1-\lambda)/\sigma^2}$$

and the limiting Pitman efficiency for these shift alternatives is

$$e^P_{U_{YX},t} = \frac{\mathcal{E}^2_{U_{YX}}}{\mathcal{E}^2_t} = 12\sigma^2 \left[\int_{-\infty}^{\infty} \psi^2(x)dx\right]^2$$

where $\psi(x) = d\Psi(x)/dx$ is the density for Ψ. This is the same expression as in equation (15.9), (see table 15.5), for the one sample Wilcoxon signed rank test Pitman efficiency relative to the one sample t test.

This efficiency is also the limiting ratio of variances for the point estimate $\hat{\Delta}$ relative to $\bar{X} - \bar{Y}$ as shown by Hodges and Lehmann (1963)[18].

---

[19]Noether, G.E. (1955) On a theorem of Pitman. *Annals of Mathematical Statistics* **26**,64-68

[20]Hoeffding, W. (1948). A class of statistics with asymptotically normal distribution. *Annals of Mathematical Statistics* **19**, 293-325.

[21]Chernoff, H. and Savage, I.R. (1958). Asymptotic normality and efficiency of certain nonparametric test statistics. *Annals of Mathematical Statistics* **29**,972-994.

15.5 Mood and Brown Median Test for K Samples

Let samples $\{X_{ij} : \ j = 1, 2, \ldots, n_i\}$ be independent with distribution function $F_i(x)$ for $i = 1, 2, \ldots, K$. To test the hypothesis

$$H : \ F_1 = F_2 = \cdots = F_K \text{ versus } A : \text{ not all } F_i \text{ equal}, \tag{15.12}$$

Brown and Mood (1948)[22], (1951)[23] proposed the K sample median test which rejects H in favor of A for large values of

$$B^2(\mathbf{M}) = \frac{N(N-1)}{a(N-a)} \sum_{i=1}^{K} \left(M_i - \frac{n_i a}{N} \right)^2 / n_i$$

where $N = \sum_{i=1}^{K} n_i$, and $\mathbf{M} = (M_1, M_2, \ldots, M_K)$ are the numbers in each sample that exceed the median of the pooled sample, $a = \sum_{i=1}^{K} M_i$.

15.5.1 The Exact Null Distrbution of B^2

To take into account the possibility of ties, consider the discrete case where the samples take on the values $z_1 < z_2 < \cdots < z_c$ with probabilities

$$P_H(X_{ij} = z_r) = p_r, \quad r = 1, 2, \ldots, c \tag{15.13}$$

where $\sum_{r=1}^{c} p_r = 1$. We can construct a distribution free test of H by conditioning on the sufficient statistic $\mathbf{T} = (T_1, T_2, \ldots, T_c)$ where

$$T_r = \sum_{i=1}^{K} \sum_{j=1}^{n_i} I[X_{ij} = z_r,] \quad r = 1, 2, \ldots, c$$

is the total number of observations equal to z_r. Given $\mathbf{T} = (t_1, t_2, \ldots, t_c) = \mathbf{t}$, define the pooled sample median by

$$\tilde{z} = \begin{cases} z_s & \text{if } \sum_{r=1}^{s} t_r \geq N/2 \text{ and } \sum_{r=s}^{c} t_r \geq N/2 \\ (z_s + z_{s+1})/2 & \text{if } \sum_{r=1}^{s} t_r = N/2 \text{ and } \sum_{r=s+1}^{c} t_r = N/2 \end{cases} .$$

[22]Brown, G.W. and Mood, A.M. (1948). Homogenity of several samples. *The American Statistician* **2** 22.

[23]Brown, G.W. and Mood, A.M. (1951). On median tests for linear hypotheses. *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability* University of California Press, Berkeley, California, pp 159-166.

Then the counts above the median are $M_i = \sum_{j=1}^{n_i} I[X_{ij} > \tilde{z}]$. We have for $a = \sum_{i=1}^{K} m_i$,

$$P_H(\mathbf{M} = (m_1, m_2, \ldots, m_K)|\mathbf{T} = (t_1, t_2, \ldots, t_c)) = \frac{\binom{n_1}{m_1}\binom{n_2}{m_2}\cdots\binom{n_K}{m_K}}{\binom{N}{a}} .$$

We can calculate the exact P-value by enumeration

$$\hat{\alpha} = \sum_{\mathbf{u}\in\mathcal{R}} \prod_{i=1}^{K} \frac{\binom{n_i}{u_i}}{\binom{N}{a}}$$

where $\mathbf{u} = (u_1, u_2, \ldots u_K)$ and

$$\mathcal{R} = \{\mathbf{u} : \ u_i \text{ integer}, 0 \le u_i \le n_i, \ \sum_{i=1}^{K} u_i = a, \ B^2(\mathbf{u}) \ge B^2(\mathbf{M})\} .$$

The more efficient approach of Jorn and Klotz (2002)[24] uses the equivalent statistic

$$V(\mathbf{M}) = \sum_{i=1}^{K} M_i^2/n_i$$

where

$$B^2(\mathbf{M}) = \frac{N(N-1)}{a(N-a)}\left(V(\mathbf{M}) - \frac{a^2}{N}\right) .$$

If we write $N_k = \sum_{i=1}^{k} n_i$, $V_k = \sum_{i=1}^{k} M_i^2/n_i$, and $a_k = \sum_{i=1}^{k} M_i$ for $k = 1, 2, \ldots, K$ then for

$$Q_k(v_k|a_k) = P_H(V_k \ge v_k|\mathbf{t})$$

we have the convolution formula

$$Q_k(v_k|a_k) = \sum_{m_k=\underline{L}_k}^{\overline{L}_k} Q_{k-1}(v_k - m_k^2/n_k|a_k - m_k)\frac{\binom{n_k}{m_k}\binom{N_{k-1}}{a_k-m_k}}{\binom{N_k}{a_k}}$$

where $\underline{L}_k = \max(0, a_k - N_{k-1})$ and $\overline{L}_k = \min(a_k, n_k)$. For $k = 1$ we start with the indicator function $Q_1(v_1|a_1) = I[a_1^2/n_1 \ge v_1]$.

[24]Jorn, H. and Klotz, J. (2002). Exact distribution of the K sample Mood and Brown median test. *Nonparametric Statistics* **14**, 249-257.

For contrasts, we can adapt the multiple comparison method of Scheffé (1959)[25] using contrasts of the form

$$\hat{\phi} = \sum_{i=1}^{K} C_i M_i / n_i, \text{ where } \sum_{i=1}^{K} C_i = 0 \ .$$

We have the following

Theorem 15.1 *Under the hypothesis, the probability is $1-\alpha$ that simultaneously for all contrasts*

$$-\left[h_\alpha \, Var(\hat{\phi})\right]^{1/2} < \hat{\phi} < \left[h_\alpha \, Var(\hat{\phi})\right]^{1/2}$$

where

$$Var(\hat{\phi}) = \frac{a(N-a)}{N(N-1)} \sum_{i=1}^{K} \frac{C_i^2}{n_i}, \quad a = \sum_{i=1}^{K} M_i, \quad N = \sum_{i-1}^{K} n_i$$

and h_α satisfies $P_H(B^2 \geq h_\alpha \, |\mathbf{t}) = \alpha$.

Proof: Since $\sum_{i=1}^{K} C_i = 0$, by Schwartz inequality

$$\hat{\phi}^2 = \left(\sum_{i=1}^{K} \frac{C_i M_i}{n_i}\right)^2 = \left(\sum_{i=1}^{K} \frac{C_i}{\sqrt{n_i}} \left(\frac{(M_i - n_i a/N)}{\sqrt{n_i}}\right)^2\right)$$

$$\leq \left(\sum_{i=1}^{K} \frac{C_i^2}{n_i}\right) \left(\sum_{i=1}^{K} \frac{(M_i - n_i a/N)^2}{n_i}\right)$$

$$= \left(\frac{a(N-a)}{N(N-1)} \sum_{i=1}^{K} \frac{C_i^2}{n_i}\right) \left(\frac{N(N-1)}{a(N-a)} \sum_{i=1}^{K} \left(M_i - \frac{n_i a}{N}\right)^2 / n_i\right) = \mathrm{Var}(\hat{\phi}) B^2$$

and

$$P_H(\hat{\phi}^2 < h_\alpha \mathrm{Var}(\hat{\phi}) \, |\mathbf{t}) \geq P_H(B^2 \mathrm{Var}(\hat{\phi}) < h_\alpha \mathrm{Var}(\hat{\phi}) \, |\mathbf{t}) = 1 - \alpha \ . \ \blacksquare$$

The program **Mood.cpp** in appendix N calculates the P-value for the Mood and Brown test with an options for contrasts and methods for data entry.

[25] Scheffé, H. (1959). *The Analysis of Variance.* John Wiley and Sons, New York.

For eaample if we compile the file **Mood.cpp** with the command **g++ -o Mood Mood.cpp** for the gnu C++ compiler and then execute it with **Mood** then, for the choices made, we obtain the following output for data in file **Mood.dat**, which has 8 lines for the 8 samples, and selecting a contrast with coefficients $(0, 0, 2, 0, -1, 0, -1, 0)$:

```
Do you wish to enter data vaues or counts?
Type V for data values or C for counts : v
Do you wish to enter data from the keyboard or from a file?
Type K for keyboard or F for file : f
Enter input data file name: Mood.dat
Data matrix:
2 2.8 3.3 3.2 4.4 3.6 1.9 3.3 2.8 1.1
3.5 2.8 3.2 3.5 2.3 2.4 2 1.6
3.3 3.6 2.6 3.1 3.2 3.3 2.9 3.4 3.3 3.2
3.2 3.3 3.2 2.9 3.3 2.5 2.6 2.8
2.6 2.6 2.9 2 2 2.1
3.1 2.9 3.1 2.5
2.6 2.2 2.2 2.5 1.2 1.2
2.5 2.4 3 1.5

Sample counts m[i] of values above pooled median,
and sample sizes n[i], for i=1,2,...,8.

 #i |   1    2    3    4    5    6    7    8  | Total
-------------------------------------------------------
m[i]|   5    3    9    5    1    3    0    1  |   27
-------------------------------------------------------
n[i]|  10    8   10    8    6    4    6    4  |   56
-------------------------------------------------------

Median of pooled sample is 2.8 .

Do you wish to write answers to a file?
Type y)es or n)o : n

The Mood & Brown chi square statistic Chi^2= 17.696
Equivalently, V=M[1]^2/n[1]+...+M[K]^2/n[K]= 17.517
```

```
The P-value P[V>=17.517]= 0.0068961050168
for K=8, n=(10, 8, 10, 8, 6, 4, 6, 4), and  a=27.

count=384847

Program time : 0 seconds.
Program ticks: 290000 ticks.

Do you wish to enter a contrast?
Please enter y)es or n)o : y
The values of M[i]-a*n[i]/N are :
 0.1786 -0.8571   4.179   1.143  -1.893   1.071  -2.893 -0.9286

Enter 8 constants that add to zero : 0 0 2 0 -1 0 -1 0
phi= 1.633
Confidence probability for this contrast is : 0.965755
Do you wish to enter a contrast?
Please enter y)es or n)o : n
```

15.5.2 Large Sample Null Distribution Approxination

As $N \to \infty$ with $n_i/N \to \lambda_i$, where $0 < \lambda_i < 1$ and $\sum_{i=1}^{K} \lambda_i = 1$, we have

$$B^2(\mathbf{M}) = \frac{N(N-1)}{a(N-a)} \sum_{i=1}^{K} \left(M_i - \frac{n_i a}{N} \right)^2 / n_i \xrightarrow{d} \chi^2_{K-1}(0)$$

under the hypothesis. This follows from the limiting normal distribution of

$$\mathbf{Z} = \left(\frac{(M_1 - n_1 a/N)}{\sqrt{n_1}}, \frac{(M_2 - n_2 a/N)}{\sqrt{n_2}}, \ldots, \frac{(M_K - n_K a/N)}{\sqrt{n_K}} \right)^T \xrightarrow{d} \mathcal{N}_K(\mathbf{0}, \mathbf{\Sigma})$$

where the $K \times K$ matrix of rank $K-1$ is

$$\mathbf{\Sigma} = \frac{1}{4} \begin{pmatrix} 1-\lambda_1 & -\sqrt{\lambda_1\lambda_2} & \cdots & -\sqrt{\lambda_1\lambda_K} \\ -\sqrt{\lambda_2\lambda_1} & 1-\lambda_2 & \cdots & -\sqrt{\lambda_2\lambda_K} \\ \vdots & \vdots & \ddots & \vdots \\ -\sqrt{\lambda_K\lambda_1} & -\sqrt{\lambda_K\lambda_2} & \cdots & 1-\lambda_K \end{pmatrix}$$

since

$$\mathrm{Var}_H\left(\frac{M_i}{\sqrt{n_i}}\right) = \frac{a(N-a)(N-n_i)}{N^2(N-1)} \longrightarrow \frac{1}{4}(1-\lambda_i)\ ,$$

and

$$\mathrm{Cov}_H\left(\frac{M_i}{\sqrt{n_i}}, \frac{M_j}{\sqrt{n_j}}\right) = -\frac{a(N-a)}{N^2(N-1)}\sqrt{n_i n_j} \longrightarrow -\frac{1}{4}\sqrt{\lambda_i \lambda_j}\ .$$

Then using proposition 10.7 in section 10.8, and $\frac{1}{4}\mathbf{\Sigma}^- = \mathbf{I}_K$, the $K \times K$ identity matrix, we have

$$B^2 = \left(\frac{N(N-1)}{a(N-a)}\right)\mathbf{Z}^T\mathbf{I}_K\mathbf{Z} = \left(\frac{N(N-1)}{a(N-a)}\right)\frac{1}{4}\mathbf{Z}^T\mathbf{\Sigma}^-\mathbf{Z} \xrightarrow{d} 4\frac{1}{4}\chi^2_{K-1}(0)\ .$$

15.5.3 Liniting Pitman efficiency of B^2

If we compare B^2 against the $\mathcal{F}$ test for the analysis of variance one way layout for shift alternatives $F_i(x) = \Psi(x-\mu_i)$, $i = 1, 2, \ldots, K$ with $\mu_i = O(1/\sqrt{N})$ as $N \to \infty$, we obtain the same expression as for the two sample comparison, namely

$$e^P_{B^2,\mathcal{F}} = 4\sigma^2\psi^2(0)$$

where ψ is the density for Ψ. See table 15.6.

15.6 The Kruskal Wallis H Test

As in the discussion for the Mood and Brown K sample test, let the samples $\{X_{ij} :\ j = 1, 2, \ldots, n_i\}$ be independent with c.d.f $F_i(x)$ for $i = 1, 2, \ldots, K$. Kruskal (1952)[26] and Kruskal and Wallis (1952)[27] proposed a test for the K sample hypothesis (15.12) based on rejection for large values of the statistic

$$H = \frac{12}{N(N+1)[1-\gamma/(N^3-N)]}\sum_{k=1}^{K}\left(R_{k+} - n_i\frac{(N+1)}{2}\right)^2/n_i$$

[26]Kruskal, W.H. (1952). A nonparametric test for the several sample problem. *Annals of Mathematical Statistics* **23**, 525-540

[27]Kruskal, W.H. and Wallis, W.A. (1952). Use of ranks on one criterion analysis of variance. *Journal of the American Statistical Association* **47**, 583-621.

where

$$R_{k+} = \sum_{i=1}^{n_i} R(X_{ij}), \quad \gamma = \sum_{r=1}^{c} (t_r^3 - t_r) \ ,$$

$R(X_{ij})$ is the rank of X_{ij} in the pooled sample of size $N = \sum_{i=1}^{K} n_i$, and t_r is the number tied for the rth largest observation with c distinct values.

When $K = 2$ the test reduces to the two sided two sample Wilcoxon rank sum test.

15.6.1 Null Distribution of H

Kruskal and Wallis (1952)[27] discuss the exact distribution and gave tables for $K = 3$ and $n_1, n_2, n_3 \leq 5$. More extensive tables are given by Iman et. al. (1975)[28].

For large samples, Kruskal an Wallis (1952)[27] also discuss the $\chi^2_{K-1}(0)$ approximation of the null distribution.

15.6.2 Null Distribution of H with Ties

If the distribution is discrete with sample values taking on the values $z_1 < z_2 < \cdots < z_c$ with probability

$$P(X_{ij} = z_r) = p_{ir} \text{ for } j = 1, 2, \ldots, n_i \text{ and } r = 1, 2, \ldots, c \ .$$

The hypothesis is then $p_{ir} = p_r$ for $i = 1, 2, \ldots, K$ as in equation (15.13) for the Mood and Brown K sample test. Then for the counts

$$U_{ir} = \sum_{j=1}^{n_i} I[X_{ij} = z_r] \text{ for } i = 1, 2, \ldots, K \text{ and } r = 1, 2, \ldots, c$$

and the $K \times c$ matrix of these counts

$$\mathbf{U} = \begin{pmatrix} \mathbf{U}^{(1)} \\ \mathbf{U}^{(2)} \\ \vdots \\ \mathbf{U}^{(K)} \end{pmatrix} = \begin{pmatrix} U_{11} & U_{12} & \cdots & U_{1c} \\ U_{21} & U_{22} & \cdots & U_{2c} \\ \vdots & \vdots & \ddots & \vdots \\ U_{K1} & U_{K2} & \cdots & U_{Kc} \end{pmatrix}$$

[28]Iman, R.L., Quade, D., and Alexander, D.A. (1975). Exact probability levels for the Kruskal-Wallis Test. *Selected Tables in Mathematical Statistics* **3** 329-384.

we have

$$P_H(\mathbf{U} = \mathbf{u}) = \left[\prod_{i=1}^{K} \frac{n_i!}{u_{i1}!u_{i2}!\cdots u_{ic}!}\right] p_1^{t_1} p_2^{t_2} \cdots p_c^{t_c}$$

where $t_r = \sum_{i=1}^{K} u_{ir}$. Under the hypothesis $\mathbf{T} = (T_1, T_2, \ldots, T_c)$ where $T_r = \sum_{i=1}^{K} U_{ir}$ is sufficient for $\mathbf{p} = (p_1, p_2, \ldots, p_c)$,

$$P_H(\mathbf{T} = \mathbf{t}) = \frac{N!}{t_1!t_2!\cdots t_c!} p_1^{t_1} p_2^{t_2} \cdots p_c^{t_c}$$

and we can condition on $\mathbf{T}$ to obtain a parameter free distribution

$$P_H(\mathbf{U} = \mathbf{u}|\mathbf{T} = \mathbf{t}) = \left[\prod_{i=1}^{K} \frac{n_i!}{u_{i1}!u_{i2}!\cdots u_{ic}!}\right] / \frac{N!}{t_1!t_2!\cdots t_c!} \ .$$

If we use average ranks for the rth largest value given by

$$a_r = t_1 + t_2 + \cdots + t_{r-1} + (t_r + 1)/2$$

then the value of the Kruskal Wallis statistic is

$$H(\mathbf{u}) = \frac{12}{N(N+1)[1 - \gamma/(N^3 - N)]} \sum_{k=1}^{K} (R_{k+}(\mathbf{u}^{(k)}) - n_k(N+1)/2)^2/n_i$$

where the value of the sum of the average ranks for the ith sample is

$$R_{k+}(\mathbf{u}^{(k)}) = \sum_{r=1}^{c} u_{kr} a_r \ , \text{ and } \gamma = \sum_{r=1}^{c} (t_r^3 - t_r) \ .$$

If we observe $\mathbf{U} = \mathbf{u}_0$ then the exact P-value for the test is

$$\hat{\alpha}(\mathbf{u}_0) = \sum_{\mathbf{u} \in \mathcal{R}} I[H(\mathbf{u}) \geq H(\mathbf{u}_0)] \left[\prod_{i=1}^{K} \frac{n_i!}{u_{i1}!u_{i2}!\cdots u_{ic}!}\right] / \frac{N!}{t_1!t_2!\cdots t_c!}$$

where

$$\mathcal{R} = \{\mathbf{u} : \ 0 \leq u_{ij} \text{ integer}, \ \sum_{i=1}^{K} u_{ir} = t_r, \ \sum_{r=1}^{c} u_{ir} = n_i\}$$

with $\mathbf{t}$ and $(n_1, n_2, \ldots, n_K)$ the column and row margins of $\mathbf{u}_0$.

Klotz and Teng (1977)[29] devloped a program that enumerated all possible count matrices $\mathbf{u}$ with the given margins to calculate P-values. More recently, Jorn and Klotz slightly improved the calculation by using a convolution.

Define the equivalent statistic

$$V_K = \sum_{i=1}^{K} R_{i+}^2/n_i$$

where

$$H = \frac{12}{N(N+1)[1-\gamma/(N^3-N)]}\left[V_K - N(N+1)^2/4\right] .$$

Let

$$Q_K(v_K|\mathbf{t}) = P_H(V_k \geq v_K|\mathbf{T}=\mathbf{t}) .$$

Denoting

$$t_r^{(k)} = \sum_{i=1}^{k} u_{ir}, \quad \mathbf{t}^{(k)} = (t_1^{(k)}, t_2^{(k)}, \ldots, t_c^{(k)})$$

$$\mathbf{u}^{(k)} = (u_{k1}, u_{k2}, \ldots, u_{kc}), \quad N_k = n_1 + n_2 + \cdots + n_k, \text{ for } k = 1, 2, \ldots, K$$

we have

$$Q_k(v_k|\mathbf{t}^{(k)}) = \sum_{\mathbf{u}^{(k)} \in \mathcal{S}(n_k, \mathbf{t}^{(k)})} Q_{k-1}(v_k - R_{k+}^2(\mathbf{u}^{(k)})/n_k|\mathbf{t}^{(k)} - \mathbf{u}^{(k)}) \frac{\prod_{r=1}^{c}\binom{t_r^{(k)}}{u_{kr}}}{\binom{N_k}{n_k}} \tag{15.14}$$

where we use the average ranks for $\mathbf{t} = \mathbf{t}^{(K)}$ (not $\mathbf{t}^{(k)}$),

$$R_{k+}(\mathbf{u}^{(k)}) = \sum_{r=1}^{c} u_{kr} a_r^{(K)} , \quad a_r^{(K)} = t_1^{(K)} + t_2^{(K)} + \cdots + t_{r-1}^{(K)} + (t_r^{(K)} + 1)/2 ,$$

and

$$\mathcal{S}(n_k, \mathbf{t}^{(k)}) = \{\mathbf{u}^{(k)} : \ u_{kr} \text{ integer}, \ 0 \leq u_{kr} \leq t_r^{(k)} , \ \sum_{r=1}^{c} u_{kr} = n_k\} .$$

[29] Klotz, J. and Teng, J. (1977). One-way layout for counts and the exact enumeration of the Kruskal-Wallis H distribution with ties. *Journal of the American Statistical Association* **72**, 165-169.

We start with

$$Q_1(v_1|\mathbf{t}^{(1)}) = I[\sum_{r=1}^{c} u_{1r}a_r^{(K)} \geq v_1] \text{ where } \mathbf{t}^{(1)} = \mathbf{u}^{(1)} \ . \tag{15.15}$$

Setting up a vector $A[1, 2, \ldots, K]$ of nodes of the form

$$(v_k, Q_k(v_k|\mathbf{t}^{(k)}), \mathbf{t}^{(k)}, \mathbf{u}^{(k)}) \text{ for } k = 1, 2, \ldots, K$$

we initially set the node $A[K]$ to

$$(v_K, 0, \mathbf{t}^{(K)}, \mathbf{u}^{(K)})$$

where v_K is the observed value of V_K and $\mathbf{u}^{(K)}$ is the starting vector in lexical order in the set $\mathcal{S}(n_K, \mathbf{t}^{(K)})$. Nodes $A[k]$ for $k = K-1, K-2, \ldots, 1$ are then initially set to

$$(v_k, 0, \mathbf{t}^{(k)}, \mathbf{u}^{(k)})$$

where

$$v_k = v_{k+1} - R^2_{k+1,+}/n_{k+1} \ , \quad R^2_{k+1,+} = \sum_{r=1}^{c} u_{k+1,r}a_r^{(K)} \ , \quad \mathbf{t}^{(k)} = \mathbf{t}^{(k+1)} - \mathbf{u}^{(k+1)}$$

and $\mathbf{u}^{(k+1)}$ and $\mathbf{t}^{(k+1)}$ are obtained from $A[k+1]$ and $\mathbf{u}^{(k)}$ is the starting vector in lexical order in the set $\mathcal{S}(n_k, \mathbf{t}^{(k)})$.

After this initialization we set $Q_1(v_1|\mathbf{t}^{(1)})$ in $A[1]$ using (15.15) and then add to $Q_k(v_k|\mathbf{t}^{(k)})$ in $A[k]$ for $k = 2, 3, \ldots, K$ using equation (15.14). After each addition to $Q_k(v_k|\mathbf{t}^{(k)})$, the value of $\mathbf{u}^{(k)}$ is changed to the next largest in lexical order in $\mathcal{S}(n_k, \mathbf{t}^{(k)})$ and then $\mathbf{u}^{(k-1)}, \mathbf{u}^{(k-2)}, \ldots, \mathbf{u}^{(1)}$ are reset to the smallest in lexical order. When $\mathbf{u}^{(k)}$ is at its largest in lexical order and cannot be changed, then $Q_{k+1}(v_{k+1}|\mathbf{t}^{(k+1)}$ is added to using (15.14) and nodes $A[k], A[k-1], \ldots, A[1]$ reset in a similar way. The process ends when $\mathbf{u}^{(K)}$ is the largest in lexical order and then $Q_K(v_K|\mathbf{t})$ is the P-value.

Program **HTest.cpp** in appendix O calculates exact P-values for an array of counts **U**. For eaample, compiling with

g++ -o HTest HTest.cpp

and then executing with

HTest

we get the following output:

```
Exact P-value for the Kruskal-Wallis H test with ties
Program for small arrays of counts.
Copyright (C) Jerome Klotz and Hongsuk Jorn
University of Wisconsin and Inha University.

Enter number of rows K : 4
Enter number of columns C : 5
Enter counts by rows (4 rows, 5 columns):
Enter U[1]: 15 0 1 1 0
Enter U[2]: 15 1 1 0 1
Enter U[3]:  9 3 1 0 2
Enter U[4]: 17 1 0 0 0

4x5 Data Matrix & Margins
|  15    0    1    1    0 |  17
|  15    1    1    0    1 |  18
|   9    3    1    0    2 |  15
|  17    1    0    0    0 |  18
--------------------------------
|  56    5    3    1    3 |  68

Average Ranks:
28.5 59 63 65 67

Test statistics using average ranks:
Kruskal Wallis statistic with ties H=7.20629
  R[1,+]^2/n[1]+...+R[K,+]^2/n[K]= V=82179.6

P-value: P[ H>=7.20629 |t]= 0.0590693

Node Count = 89600

Program time : 0 seconds.
Program ticks: 100000 ticks.
```

We note that the program generates the same number of nodes as $||\mathcal{R}||$, the number of matrices $\mathbf{U}$ with these margins.

The program can take a very large amount of time for larger matrices. For

example, a 4×5 array of counts with $(n_1, n_2, n_2, n_4) = (22, 29, 27, 28)$ and $\mathbf{t} = (4, 11, 37, 36, 18)$ has $||\mathcal{R}|| = 63,646,854,206$ so that the $\chi^2_3(0)$ approximation should be used. The Benard van Elteren test in the next section can be used to calculate this by setting the number of blocks $b = 1$.

15.6.3 Limiting Pitman efficiency of the H test

If we compare H against the $\mathcal{F}$ test for the analysis of variance one way layout for shift alternatives $F_i(x) = \Psi(x - \mu_i)$, $i = 1, 2, \ldots, K$ with density $\psi(u) = d\Psi(u)/du$ and $\mu_i = O(1/\sqrt{N})$ as $N \to \infty$, we obtain the same expression as for the comparison of the two sample Wilcoxon and the t test, namely

$$12\sigma^2 \left[\int_{-\infty}^{\infty} \psi^2(u) du \right]^2 .$$

15.7 Two Way Rank Tests

15.7.1 Benard and van Elteren test

Let $\{X_{ijk} : \imath = 1, 2, \ldots, K,\ j = 1, 2, \ldots, b,\ k = 1, 2, \ldots, n_{ij}\}$ be independent with c.d.f. $F_{ij}(x)$. We consider the hypothesis of no difference between the treatments $i = 1, 2, \ldots, K$:

$$H:\ F_{ij}(x) = F_j(x) \text{ versus not all equal for some } i.$$

The test of Benard and van Elteren (1953)[30] generalizes the tests of Friedman (1937)[31], Cochran (1950)[32], Kruskal and Wallace (1952)[33] and Durban (1951)[34]. Let R_{ijk} be the average rank in the jth block over the K treatments

[30]Benard, A.A. and van Elteren, Ph. (1953). A generalization of the method of m rankings. *Proceedings Koninklijke Akademie van Wetenschappen Amsterdam*, **56**, 358-369.

[31]Friedman, M. (1937). The use of ranks to avoid the the assumption of normality implicit in the analysis of variance. *Journal of the American Statistical Association* **32**, 675-701.

[32]Cochran, W. (1950). The comparison of percentages in matched samples. *Biometrika* **37**, 256-266.

[33]Kruskal, W.H. and Wallis, W.A. (1952). Use of ranks on one criterion analysis of variance. *Journal of the American Statistical Association* **47**, 583-621.

[34]Durban, J. (1951). Incomplete blocks in ranking experiments. *British Journal of Psychology (Statistical Section)*, **4**, 85-90.

for the $n_{+j} = \sum_{i=1}^{K} n_{ij}$ observations. Define

$$R_{i++} = \sum_{j=1}^{b} \sum_{k=1}^{n_{ij}} R_{ijk}$$

$$E_H(R_{i++}) = \sum_{j=1}^{b} n_{ij}(n_{j} + 1)/2$$

$$U_i = (R_{i++} - E_H(R_{i++})), \quad \mathbf{U} = (U_1, U_2, \ldots, U_K)^T,$$

$$\sigma_{ii} = \mathrm{Var}_H(R_{i++}) = \sum_{j=1}^{b} n_{ij}(n_{+j} - n_{ij})(n_{+j} + 1)(1 - \gamma_j/(n_{+j}^3 - n_{+j}))/12,$$

$$\sigma_{ii'} = \mathrm{Cov}_H(R_{i++}, R_{i'++}) = -\sum_{j=1}^{b} n_{ij} n_{i'j}(n_{+j} + 1)(1 - \gamma_j/(n_{+j}^3 - n_{+j}))/12,$$

The tie correction factors are $\gamma_j = \sum_{r=1}^{c_j}(t_{jr}^3 - t_{jr})$ with t_{jr} the total number in the j th block tied for the r th largest value among the c_j distinct block values and

$$\mathbf{\Sigma} = (\sigma_{ii'} : i, i' = 1, 2, \ldots K) \ .$$

The statistic, which is invariant under the choice of a generalized inverse $\mathbf{\Sigma}^-$ that satisfies $\mathbf{\Sigma}\mathbf{\Sigma}^-\mathbf{\Sigma} = \mathbf{\Sigma}$, is symmetric ($\mathbf{\Sigma}^- = (\mathbf{\Sigma}^-)^T$), and reflexive ($\mathbf{\Sigma}^-\mathbf{\Sigma}\mathbf{\Sigma}^- = \mathbf{\Sigma}^-$), is

$$V = \mathbf{U}^T\mathbf{\Sigma}^-\mathbf{U} \ .$$

We use a $\chi^2_{K-1}(0)$ approximation to the null distribution using a limiting joint normal distribution for normalized $\mathbf{U}$ and proposition 10.7 in section 10.8. We reject H if $V \geq \chi^2_{K-1,\alpha}(0)$ where $\chi^2_{K-1,\alpha}(0)$ is the upper α probability point.

Since $\mathbf{\Sigma}$ is of rank $K-1$, a particular and convenient generalized inverse is obtained by deleting the last row and column of $\mathbf{\Sigma}$ to get the $(K-1)\times(K-1)$ nonsingular matrix $\mathbf{\Sigma}_{11}$. Inverting it, we can use

$$\mathbf{\Sigma}^- = \begin{pmatrix} \mathbf{\Sigma}_{11}^{-1} & \mathbf{0} \\ \mathbf{0} & 0 \end{pmatrix}, \text{ where } \mathbf{\Sigma} = \begin{pmatrix} \mathbf{\Sigma}_{11} & \boldsymbol{\sigma}_{12} \\ \boldsymbol{\sigma}_{21} & \sigma_{22} \end{pmatrix} .$$

Since the determinant $|\mathbf{\Sigma}| = 0$, we get

$$\begin{vmatrix} \mathbf{\Sigma}_{11} & \boldsymbol{\sigma}_{12} \\ \boldsymbol{\sigma}_{21} & \sigma_{22} \end{vmatrix} \begin{vmatrix} \mathbf{\Sigma}_{11}^{-1} & \mathbf{0} \\ \mathbf{0} & 1 \end{vmatrix} = \begin{vmatrix} \mathbf{I}_{K-1} & \boldsymbol{\sigma}_{12} \\ \boldsymbol{\sigma}_{21}\mathbf{\Sigma}_{11}^{-1} & \sigma_{22} \end{vmatrix} = \sigma_{22} - \boldsymbol{\sigma}_{21}\mathbf{\Sigma}_{11}^{-1}\boldsymbol{\sigma}_{12} = 0 \ .$$

Thus $\sigma_{22} = \boldsymbol{\sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\sigma}_{12}$ and

$$\boldsymbol{\Sigma}\boldsymbol{\Sigma}^{-}\boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\Sigma}_{11} & \boldsymbol{\sigma}_{12} \\ \boldsymbol{\sigma}_{21} & \boldsymbol{\sigma}_{21}\boldsymbol{\Sigma}_{11}^{-1}\boldsymbol{\sigma}_{12} \end{pmatrix} = \boldsymbol{\Sigma}\ .$$

Then

$$V = (U_1, U_2, \ldots, U_{K-1})\boldsymbol{\Sigma}_{11}^{-1}\begin{pmatrix} U_1 \\ U_1 \\ \vdots \\ U_{K-1} \end{pmatrix}\ .$$

For an example, consider the values

X_{ijk}	$j=1$	2	3	4
$i=1$	3 3 5	2 1	3 3 7	2 2 1
2	4 6 3		5 2	1 7
3	5 1 2 4	7 6 8 1	4 3 5	8 9

We calculate

R_{ijk} n_{ij}	$j=1$	2	3	4	R_{i++}	$E(R_{i++})$	U_i
$i=1$	4 4 3 8.5	3 1.5 2	3 3 3 8	3.5 3.5 3 1.5	43.5	49	-5.5
2	6.5 10 3 4	$-$ 0	6.5 1 2	1.5 5 2	34.5	35.5	1.0
3	8.5 1 2 4 6.5	5 4 6 4 1.5	5 3 3 6.5	6 7 2	62.0	57.5	4.5
$\gamma_j,\ n_{+j}$ || sum	36, 10	6, 6	30, 8	12, 7	140	140	0

Then

$$\mathbf{\Sigma}_{11} \doteq \begin{pmatrix} 41.37797615 & -16.03928572 \\ -16.03928572 & 33.44285714 \end{pmatrix}, \quad \mathbf{U} = \begin{pmatrix} -5.5 \\ 1.0 \\ 4.5 \end{pmatrix},$$

and

$$V \doteq (-5.5,\ 1.0) \begin{pmatrix} 41.37797615 & -16.03928572 \\ -16.03928572 & 33.44285714 \end{pmatrix}^{-1} \begin{pmatrix} -5.5 \\ 1.0 \end{pmatrix} \doteq 0.77813\,.$$

The P-value, using a $\chi^2_2(0)$ approximation, is

$$\hat{\alpha} \doteq P(\chi^2_2(0) \geq 0.77813) \doteq 0.67769$$

which is not significant.

If $n_{ij} = 1$ for all $i = 1, 2, \ldots, K$ and $j = 1, 2, \ldots, b$, then V reduces to the Friedman statistic

$$V = \frac{12}{bK(K+1)\{1 - \gamma/(b(K^3 - K))\}} \sum_{i=1}^{K} \left(R_{i+} - \frac{b(K+1)}{2} \right)^2$$

where $\gamma = \sum_{j=1}^{b} \gamma_j$.

15.7.2 Friedman's test

Appendix Q gives a program to calculate approximate and small sample exact P-values for Friedman's test. For example, if we compile the program (**g++ -o Friedman Friedman.cpp**) and execute it (**Friedman**) and type the file name **Leh.data** with the following values:

4	7					
251	126	49	45	233	291	1385
207	180	123	85	232	208	1204
167	104	63	147	233	158	1611
301	120	186	100	250	183	1913

.

Then the output is:

```
Exact and approximate P-value for Friedman's test by Jerome Klotz.

Enter input data file name: Leh.data
Input Data X[i,j] for i=1,2,...,4 (treatments), j=1,2,...,7 (blocks).
   251    126     49     45    233    291   1385
   207    180    123     85    232    208   1204
   167    104     63    147    233    158   1611
   301    120    186    100    250    183   1913

Average Ranks R[i,j]                              | R[i+]
     3      3      1      1    2.5      4      2 | 16.5
     2      4      3      2      1      3      1 | 16
     1      1      2      4    2.5      1      3 | 14.5
     4      2      4      3      4      2      4 | 23

Friedman statistic (corrected for ties) :3.69565
Tie correction factor gamma=sum(gamma[j]) :6
Approximate P-value : P[Chi Square > 3.69565 | 3 d.f. ]=0.296259

Permuting Product{(K!)/(t[j][1]!...t[j][c[j]]!) : j=1,...,b-1}=95551488
columns and calculating statistics.
If this number is large, it may take a while.

Tie counts {t[j][r] :r=1,2,...,c[j]} for columns 1,2,...,7 :
(1, 1, 1, 1),(1, 1, 1, 1),(1, 1, 1, 1),(1, 1, 1, 1),(1, 2, 1),
(1, 1, 1, 1),(1, 1, 1, 1) .
Permutation counts for columns 1,2,...,6 :(24, 24, 24, 24, 12, 24) .
Equivalent Statistic Q=1267.5
Exact P-value : 30121268/95551488=0.315236 .
```

The Friedman test furthur reduces to Cochran's statistic for dichotomous responses ($X_{ij} \in \{0,1\}$). For this case $t_{j1} = K - X_{+j}$, $t_{j2} = X_{+j}$,

$$\left(1 - \frac{\gamma}{b(K^3 - K)}\right) = \frac{3}{b(K^2-1)} \sum_{j=1}^{b} X_{+j}(K - X_{+j})$$

$$R_{i++} = \frac{b(K+1)}{2} + \frac{K}{2}(X_{i+} - X_{++}/K)^2$$

and V simplifies to Cochran's form

$$V = \frac{K(K-1)}{\sum_{j=1}^{b} X_{+j}(K - X_{+j})} \sum_{i=1}^{K} (X_{i+} - X_{++}/K)^2 \ .$$

15.7.3 Durban's test

For the balanced incomplete block test of Durban (1951)[35] define

K the number of treatments.

b the number of blocks.

d the number of observations per block, $d < K$.

a the number of times each treatment occurs

λ the number of blocks in which the i-th and i'-th treatments occur together (the same for all pairs (i, i'), with $i \neq i'$).

The treatment and value matrices are respectively

$$\mathbf{T} = (T_{ij} : \ i = 1(1)d, \ j = 1(1)b \ ) \text{ , and } \mathbf{X} = (X_{i,j} : \ i = 1(1)d, \ j = 1(1)b \ ) \ .$$

For block j, if there is a treatment i, let $R_{i,j}$ be the average rank of the value among that block's existing treatment values and 0 if there is no such treatment. We define $R_{i,+} = \sum_{j=1}^{b} R_{i,j}$ and $U_i = R_{i,+} - a(d+1)/2$.
The variance, covariance matrix is

$$\mathbf{\Sigma}^{K \times K} = (\sigma_{i,i'} : \ i, i' = 1(1)K)$$

where

$$Var(R_{i,+}) = \sigma_{i,i} = \sum_{j=1}^{b} n_{i,j}(d - n_{i,j})(d+1)(1 - \gamma_j/(d^3 - d))/12$$

$$Cov(R_{i,+}, R_{i',+}) = \sigma_{i,i'} = -\sum_{j=1}^{b} n_{i,j} n_{i',j}(d+1)(1 - \gamma_j/(d^3 - d))/12$$

[35]Durban, J. (1951). Incomplete blocks in ranking experiments. *British Journal of Psychology (Statistical Section)* **4**, 85-90.

with t_k for $k = 1, 2, \ldots, c_j$ the numbers tied in block j, a total of c_j different values, and $\gamma_j = \sum_{k=1}^{c_j}(t_k^3 - t_k)$ is the tie correction factor. The value $n_{i,j} = 1$ if treatment i is in block j with $n_{i,j} = 0$ otherwise, $i = 1(1)K$, $j = 1(1)b$.

To define Durban's statistic, let

$$\mathbf{U}^{K\times 1} = (U_1, U_2, \ldots, U_K)^T, \quad \mathbf{V}^{(K-1)\times 1} = (U_1, U_2, \ldots, U_{K-1})^T$$

$$\boldsymbol{\Sigma}_{1,1}^{(K-1)\times(K-1)} = (\sigma_{i,i'} : \ i, i' = 1(1)(K-1))$$

$$\boldsymbol{\Sigma}_{1,1} = \mathbf{L}\mathbf{L}^T$$

where $\mathbf{L}^{(K-1)\times(K-1)}$ is the lower triangular Choleski decomposition of $\boldsymbol{\Sigma}_{1,1}$ given by

$$\mathbf{L} = \begin{pmatrix} r_{1,1} & 0 & 0 & \ldots & 0 \\ r_{2,1} & r_{2,2} & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ r_{(K-1),1} & r_{(K-1),2} & r_{(k-1),3} & \ldots & r_{(K-1),(K-1)} \end{pmatrix}$$

and

$$r_{i,i} = (\sigma_{i,i} - \sum_{k=1}^{i-1} r_{i,k}^2)^{1/2}, \ r_{i,i'} = (\sigma_{i,i'} - \sum_{k=1}^{i'-1} r_{i,k} r_{i',k})/r_{i',i'}$$

with $\mathbf{W}$ obtained by solving the equation

$$\mathbf{L}\mathbf{W} = \mathbf{V}.$$

Then Durban's statistic is

$$Q = \mathbf{U}^T\boldsymbol{\Sigma}^-\mathbf{U} = \mathbf{V}^T\boldsymbol{\Sigma}_{1,1}^{-1}\mathbf{V} = \mathbf{W}^T\mathbf{W} \tag{15.16}$$

where $\boldsymbol{\Sigma}^-$ is a generalized inverse of $\boldsymbol{\Sigma}$ that satisfies $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^-\boldsymbol{\Sigma} = \boldsymbol{\Sigma}$.

We can verify equation (15.16) by showing that a generalized inverse

$$\boldsymbol{\Sigma}^- = \begin{pmatrix} \boldsymbol{\Sigma}_{1,1}^{-1} & \mathbf{0} \\ \mathbf{0}^T & 0 \end{pmatrix}$$

where $\mathbf{0}^{(K-1)\times 1} = (0, 0, \ldots, 0)^T$. We have $\boldsymbol{\Sigma}\boldsymbol{\Sigma}^-\boldsymbol{\Sigma} =$

$$\begin{pmatrix} \boldsymbol{\Sigma}_{1,1} & \boldsymbol{\sigma}_{1,2} \\ \boldsymbol{\sigma}_{2,1} & \sigma_{2,2} \end{pmatrix} \begin{pmatrix} \boldsymbol{\Sigma}_{1,1}^{-1} & \mathbf{0} \\ \mathbf{0}^T & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{\Sigma}_{1,1} & \boldsymbol{\sigma}_{1,2} \\ \boldsymbol{\sigma}_{2,1} & \sigma_{2,2} \end{pmatrix} = \begin{pmatrix} \boldsymbol{\Sigma}_{1,1} & \boldsymbol{\sigma}_{1,2} \\ \boldsymbol{\sigma}_{2,1} & \boldsymbol{\sigma}_{2,1}\boldsymbol{\Sigma}_{1,1}^{-1}\boldsymbol{\sigma}_{1,2} \end{pmatrix} = \boldsymbol{\Sigma} \ .$$

provided $\sigma_{2,2} = \boldsymbol{\sigma}_{2,1}\boldsymbol{\Sigma}_{1,1}^{-1}\boldsymbol{\sigma}_{1,2}$. Here $\boldsymbol{\sigma}_{2,1} = \boldsymbol{\sigma}_{1,2}^T$. Since $\boldsymbol{\Sigma}$ is singular

$$0 = \begin{vmatrix} \boldsymbol{\Sigma}_{1,1} & \boldsymbol{\sigma}_{1,2} \\ \boldsymbol{\sigma}_{2,1} & \sigma_{2,2} \end{vmatrix} \begin{vmatrix} \boldsymbol{\Sigma}_{1,1}^{-1} & -\boldsymbol{\Sigma}_{1,1}^{-1}\boldsymbol{\sigma}_{1,2} \\ \mathbf{0}^T & 1 \end{vmatrix} = \begin{vmatrix} \mathbf{I} & \mathbf{0} \\ \boldsymbol{\Sigma}_{1,1}^{-1}\boldsymbol{\sigma}_{2,1} & (\sigma_{2,2} - \boldsymbol{\sigma}_{2,1}\boldsymbol{\Sigma}_{1,1}^{-1}\boldsymbol{\sigma}_{1,2}) \end{vmatrix}$$

$$= (\sigma_{2,2} - \boldsymbol{\sigma}_{2,1}\boldsymbol{\Sigma}_{1,1}^{-1}\boldsymbol{\sigma}_{1,2})\,|\mathbf{I}|$$

completing the proof since, for the identity, $|\mathbf{I}| = 1$.

For the case of no ties ($\gamma_j = 0$ for all $j = 1(1)b$), Durban's statistic simplifies to

$$Q = \frac{12(K-1)}{aK(d-1)(d+1)} \sum_{i=1}^{K} \left(R_{i,+} - \frac{a(d+1)}{2} \right)^2 . \tag{15.17}$$

Equation (15.16) reduces to equation (15.17) for no ties since the $(K-1) \times (K-1)$ matrix

$$\boldsymbol{\Sigma}_{1,1} = \frac{a(d-1)(d+1)}{12} \begin{pmatrix} 1 & -1/(K-1) & \dots & -1/(K-1) \\ -1/(K-1) & 1 & \dots & -1/(K-1) \\ \vdots & \vdots & \ddots & \vdots \\ -1/(K-1) & -1/(K-1) & \dots & 1 \end{pmatrix}$$

$$\boldsymbol{\Sigma}_{1,1}^{-1} = \frac{12(K-1)}{a(d-1)(d+1)K} \left(\begin{pmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 1 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} (1, 1, \dots, 1) \right)$$

and

$$\mathbf{V}^T\boldsymbol{\Sigma}_{1,1}^{-1}\mathbf{V} = \frac{12(K-1)}{a(d-1)(d+1)K}\left(\sum_{i=1}^{K-1} U_i^2 + \left(\sum_{i=1}^{K-1} U_i\right)^2\right) = \frac{12(K-1)}{a(d-1)(d+1)K} \sum_{i=1}^{K} U_i^2$$

since $\sum_{i=1}^{(K-1)} U_i = -U_K$. To show this

$$\sum_{i=1}^{K} U_i = \sum_{i=1}^{K} (R_{i,+} - a(d+1)/2) = bd(d+1)/2 - Ka(d+1)/2 = 0$$

because $bd = Ka$ is the number of observations.

We use a χ^2_{K-1} distribution for the approximate P-value:

$$\hat{\alpha}(Q) \doteq P[\chi^2_{K-1} > Q] \ .$$

The program Durban.cpp in appendix R calculates exact and approximate P-values for Durban's test. We can compile it (using, for example the gnu C++ compiler) with the command

g++ -o Durban Durban.cpp

and then execute it with

Durban T X

where **T** is a treatment assignment matrix with the first row values of d and b and **X** is the corresponding value matrix. For example, if the matrices **T, X** are respectively

3	7					
1	1	3	1	2	2	4
2	3	4	6	3	5	5
4	5	7	7	6	7	6

0.465	0.602	0.875	0.423	0.652	0.536	0.609
0.343	0.873	0.325	0.987	1.142	0.409	0.417
0.396	0.634	0.330	0.426	0.989	0.309	0.931

then the output is

```
P-values for Durban's nonparametric balanced incomplete block
test by Jerome Klotz.

Treatment matrix. Entries are treatments, columns are blocks.
       1        1        3        1        2        2        4
       2        3        4        6        3        5        5
       4        5        7        7        6        7        6
Value matrix. Entries are values, columns are blocks.
   0.456    0.602    0.875    0.423    0.652    0.536    0.609
   0.343    0.873    0.325    0.987    1.142    0.409    0.417
   0.396    0.634    0.330    0.426    0.989    0.309    0.931
Value of Durban statistic is Q=7.71429 .
Approximate P-value: P[ChiSquare(6)>7.71429]=0.259792 .
For calculating the exact P-value, the total number of
permutations is 46656.
Do you wish to continue? Type Y)es or N)o :y
The exact P-value is: 14224/46656=0.30487 .
```

The C++ program **BenVanElt.cpp** in appendix P calculates the value of V. If we compile it (using, for example, the gnu C++ compiler) with the command

g++ -o BenVanElt BenVanElt.cpp

and then execute it with

BenVanElt test.data

where **test.data** is the data file for the previous example:

```
3 4

3 2 3 3
3 0 2 2
4 4 3 2

3 3 5     2 1       3 3 7   2 2 1
4 6 3               5 2     1 7
5 1 2 4   7 6 8 1   4 3 5   8 9
```

then the output is:

```
Benard van Elteren test program by Jerome Klotz.
It generalizes the Friedman, Cochran, and Durban two way rank tests.

Cell counts n[i,j] for treatment row i=1,..,3, and block j=1,..,4 .
---------------------------
           3    2    3    3
           3    0    2    2
           4    4    3    2
---------------------------
n[+,j]    10    6    8    7

Average ranks:(a[j,r] : r=1,..,c[j]), j=1,..,4
-----------------------------------------------
(1, 2, 4, 6.5, 8.5, 10), (1.5, 3, 4, 5, 6), (1, 3, 5, 6.5, 8),
  (1.5, 3.5, 5, 6, 7)

Values of (R[i++],E(R[i++]),R[i++]-E(R[i++])) for i=1,..,3.
-----------------------------------------------------------
R[i++]                43.5     34.5       62
E(R[i++])               49     33.5     57.5
R[i++]-E(R[i++])      -5.5        1      4.5

Row :{(Xijk, Rijk):k=1,..,n[ij]},i=1,..,3, j=1,..,4.
-----------------------------------------------------
1:   {(3, 4), (3, 4), (5, 8.5)},  {(1, 1.5), (2, 3)},  {(3, 3),
      (3, 3), (7, 8)},  {(1, 1.5), (2, 3.5), (2, 3.5)}
2:   {(3, 4), (4, 6.5), (6, 10)},  {}, {(2, 1), (5, 6.5)},  {(1, 1.5),
      (7, 5)}
3:   {(1, 1), (2, 2), (4, 6.5), (5, 8.5)},  {(1, 1.5), (6, 4),
      (7, 5), (8, 6)},  {(3, 3), (4, 5), (5, 6.5)},  {(8, 6), (9, 7)}

Value of Benard van Elteren statistic V= 0.778129 .

P-value by a central Chi-square approximation with K-1=2 degrees of freedom:

          P[ChiSquare(2)>0.778129]=0.677691.
```

The data file has K and b as the first entries, followed by n_{ij} in lexical order $i = 1, 2, \ldots, K$, and $j = 1, 2, \ldots, b$, and then the X_{ijk} values for $i = 1, 2, \ldots, K$, $j = 1, 2, \ldots, b$, and $k = 1, 2, \ldots, n_{ij}$ in lexical order. Whitespace is ignored.

15.7.4 Efficiency of V.

Mehra and Sarangi (1967)[36] calculate the efficiency for location alternatives.

$$F_{ij}(x) = \Psi(x - \mu_i - \eta_j)$$

when $n_{ij} = n_i$. Then for $L = \sum_{i=1}^{K} n_i$, the limiting Pitman efficiency relative to the $\mathcal{F}$ test for the two way layout as $b \to \infty$ is

$$e^P_{V,\mathcal{F}} = \frac{12\sigma^2 L}{L+1} \left(\int_{-\infty}^{\infty} \psi^2(u) du \right)^2$$

where $\sigma^2 = \int_{-\infty}^{\infty} x^2 \psi(u) du - (\int_{-\infty}^{\infty} x\psi(u) du)^2$ and $\psi(u) = d\Psi(u)/du$.

For the normal distribution and $n_{ij} = 1$ for the Friedman test,

$$e^P_{V,\mathcal{F}} = \frac{3K}{\pi(K+1)} \ .$$

When $K = 2$ the test reduces to the sign test and $e^P_{S_+,t} = 2/\pi$ for the normal distribution as given in equation (15.8) or table 15.2.

15.8 Problems

1. Another type of limiting efficiency, Bahadur efficiency, compares the ratio of sample sizes for two tests with limiting type II error β, $0 < \beta < 1$ for a fixed alternative with type I errors $\alpha \to 0$ at an exponential rate. Derive the Bahadur efficiency of the sign test relative to the t-test if $X_i : F(x) = \Phi(x - \mu)$ testing $H : \mu = 0$ versus $A : \mu > 0$.

2. Calculate $E(W_+)$ and $Var(W_+)$ for a continuous alternative $F(x)$.

3. Calculate $E(U_{YX})$ and $Var(U_{YX})$ for continuous alternatives $(F(x), G(x))$.

[36] Mehra, K.L. and Sarangi, J.(1967). Efficiency of certain rank tests for comparative experiments. *Annals of Mathematical Statistics* **38**, 90-107.

4. Derive $P_H(B = b)$ for the two sample Mood and Brown test.

5. Derive $E_H(U_{YX}|\mathbf{t})$ and $Var_H(U_{YX}|\mathbf{t})$ for the case of ties.

6. If we modify the two sample median statistic to be the number of X observations that are greater than or equal the pooled sample median, give the corresponding confidence interval for the difference in location parameters.

7. If $X_1, X_2, \ldots, X_m : F(x)$ and $Y_1, Y_2, \ldots, Y_n : G(x)$ are independent, for testing $H : F(x) = G(x)$, the control quantile statistic, for a specified integer d, $0 \leq d \leq m$, rejects in favor of $A : F(x) < G(x)$ for large values of

$$U_d = \sum_{j=1}^{n} I[Y_j < X_{(d)}] \ .$$

Give $P_H(U_d = u)$, $E_H(U_d)$, and $Var_H(U_d)$ for $F(x) = G(x)$ continuous.

8. Derive the confidence interval for a location difference $\Delta = \xi - \eta$ where $F(x) = \Psi(x - \xi)$ and $G(x) = \Psi(x - \eta)$ associated with the control quantile statistic.

9. Calculate the value of the Kruskal-Wallis H test statistic for the 8 samples of sizes $(10, 8, 10, 8, 6, 4, 6, 4)$ in file **Mood.data** using the Benard van Elteren program with one block $b = 1$.

Appendix A

Subroutine cdf.h.

Programs to calculate the incomplete beta, incomplete gamma, and hypergeometric c.d.f.'s.

```
//cdf.h file. Use #include "cdf.h" to add this file to a program.
//incomplete beta, incomplete gamma, & hypergeometric subroutines
#include <cmath>  //for log(x) and exp(x) functions
#define min(a,b) ((a)<(b)? (a):(b))
#define max(a,b) ((a)<(b)? (b):(a))
#define abs(a) ((a)<0? -(a):(a))
#define sqr(a) ((a)*(a))

namespace cdf
{

double cfrac(const double *a, int n, double z)
{ // a[0]/(z+a[1]/(z+a[2]/(z+...+(z+a[n]/z)...))) continued fraction
    double s=0;
    for(int k=n-1; k>=0; k--) s=a[k]/(z+s);
    return s;
}
double Binet(double z)// Stirling's formula error term:
// uses continued fraction from Jones, William B. and W.J. Thron(1980)
//Continued Fractions: Analytic Theory and Applications. Encyclopedia of
// Mathematics and Applications Vol II, Addison Wesley, Reading New York.
{ //Binet(z)=ln(gamma(z))-(z-1/2)ln(z)+z-0.5*ln(2pi), pi=3.141592...
```

```
    double a[ ]={1/12.0, 1/30.0, 53/210.0, 195/371.0, 22999/22737.0,
                   29944523/19733142.0, 109535241009/48264275462.0};
    return cfrac(a,7,z);
}
double G(double u)
{ //ln(1+u)-u with accuracy on [-1/2,1]
     if((u<-0.5)||(u>1.0)) return log(1.0+u)-u;
     double s=0; //on [-1/2,1] do continued fraction
     for(int k=10; k>0; k--)
     {
          double dk=(double)k, dk2=2.0*dk;
          s=sqr(dk+1.0)*u/(dk2+1.0+sqr(dk)*u/(dk2+2.0+s));
     }
     return -sqr(u)/(2.0+s);
}
double lngamma(double x)
{ //ln(gamma(x)) by Stirling's approximation with error term
     const double n=7, lnsq2pi=0.918938533204673;//0.5*ln(2pi)
     double c=x, s=1.0;
     while(c<n){ s*=c; c+=1.0;}
     s=-log(s);
     return s+(c-0.5)*log(c)-c+lnsq2pi+Binet(c);
}
double perm(double a,int k)
{ // evaluates a(a-1)...(a-k+1)
     double p=a;
     for(int i=1; i<k; i++) p*=--a;
     return p;
}
double f(double x, double a, double b)
{ //x^a(1-x)^b*Gamma(a+b)/(Gamma(a+1)Gamma(b))
    double s=a*log(x)+b*log(1-x)+lngamma(a+b)-lngamma(a+1)
                   -lngamma(b);
    return exp(s);
}
double Soper(double x, double a, double b)
{ // Soper's (1921) algorithm for incomplete Beta Ix(a,b)
      const double epsilon=1.0e-14;
```

```
      double x1=1-x, sum=0, ai=1, ck, as, v=x/x1, ab1=a+b-1;
      double a12=perm(a+2,2),b2=perm(b+1,2), ab4=perm(a+b+3,4);
      int S=(int)(b+x1*(a+b)), i=0, k;
      if (S>0) do { sum+=ai; i++; ai*=v*(b-i)/(a+i); }
                  while((abs(ai/sum)>epsilon)&&(i<S));
      if(i==S) { k=0; ck=ai*x1; as=a+S;
                   do { sum+=ck; k++; ck*=x*(ab1+k)/(as+k); }
                   while(abs(ck/sum)>epsilon); }
      return sum*f(x,a+2,b+2)*a12*b2/ab4/sqr(x*x1)/x1;
}
double icbeta(double x, double a, double b)
{ //incomplete beta function Ix(a,b)
      if(x<=0)  return 0;
      if(x>=1.0) return 1.0;
      if((a>1.0)&&(b>1.0)) {
          if(x<=a/(a+b)) return Soper(x,a,b);
          else return 1.0-Soper(1-x,b,a); }
      else {
          double c=perm(a+2,3)*perm(b+1,2)/perm(a+b+3,4);
          double fxab=c*f(x,a+2,b+2)/sqr(x*(1-x));
          return fxab*(1-x*(a+b)/b)/a+icbeta(x,a+1,b+1); }
}
double lnxf(double x, double a)
{ // ln(x^ae^{-x}/gamma(a))
      double u=(x-a)/a;
      return a*G(u)+G(a)+(a+1)*log(a)-lngamma(2+a);
}
double icgamma(double x, double a)  //incomplete gamma
{ // integral(0,x] (x^{a-1}e^{-x}dx/Gamma(a)
      double d0=-708.41, epsilon=1.0e-14s,d,c,uk,ak,fk;
      if(x<=0) return 0;
      else
      {
          d=lnxf(x,a);
          if(d<d0) d=0; else d=exp(d);
          if((x<a)||(x<1.0)) {       //do series
              ak=a; uk=1; s=1;
              while(abs(uk/s)>epsilon) { ak++; uk*=x/ak; s+=uk;}
```

```
            return (s*d/a); }
        else {                  //do continued fraction
            c=0;
            for(int k=30; k>0; k--)
            { fk=(double)k; c=fk/(x+c); c=(fk-a)/(1.0+c); }
            c=1.0/(x+c);
            return (1.0-c*d); }
    }
}
double p_(double x, double N, double D, double n)
{ //hypergeometric density
    const double epsilon=1.0e-10;
    double L=max(0,n+D-N),U=min(n,D);
    if(((x+epsilon)<L)||((x-epsilon)>U) return 0;
    double s=lngamma(N-D+1)-lngamma(N+1)+lngamma(D+1)-lngamma(D-x+1);
    s+=lngamma(N-n+1)-lngamma(x+1)+lngamma(n+1)
    -lngamma(n-x+1)-lngamma(N-n-D+x+1);
    return exp(s);
}
double sum(double x, double N, double D, double n)
{
    const double epsilon=1.0e-14;
    double dk=1, s=1, ak=1;
    double L=max(0,n+D-N);
    while((dk<(x-L+0.5))&&((ak/s)>epsilon))
    {
       ak*=(1+x-dk)/(n-x+dk)*(N-D-n+x+1-dk)/(D-x+dk);
       s+=ak; dk++;
    }
    return s;
}

double HyperG(double x, double N, double D, double n)
{ //hypergeometric c.d.f
    double L=max(0,n+D-N), U=min(n,D);
    if (x<L) return 0;
    if (x>=U) return 1;
    if(x>(n+1)/(N+1)*(D+1)) return 1-HyperG(D-x-1,N,D,N-n);
```

```
    else return p_(x,N,D,n)*sum(x,N,D,n);
}

}//end namespace cdf
```

Appendix B

C++ subroutine normal.h

The following C++ subroutine calculates the standard normal c.d.f.

```
//normal.h file. Use  #include "normal.h"  to add to a C++ program.
//Subroutines for the standard normal N(0,1) c.d.f. Phi(x) .
#include <cmath>
#define abs(a) ((a)<0? -(a):(a))
#define sqr(a) ((a)*(a))

double f(double x) // Standard normal N(0,1) p.d.f.
{
   const double lnsq2pi=0.918938533204673; //0.5*ln(2pi)
   return exp(-0.5*sqr(x)-lnsq2pi);
}
double Phi(double x) // Standard normal N(0,1) c.d.f.
{
   int k, n=40;
   const double a=2.8, L=5.566E-16, U=8.13;
   double s=1, c=0,x2=sqr(x),u=1;
   if(abs(x)<L) return 0.5;
   if(x<-U) return 0;
   if(x>U) return 1.0;
   if(abs(x)<a) //do series
   {
      for(k=1; k<=n; k++) {  u*=x2/(2.0*k+1.0);  s+=u; }
      return 0.5+x*f(x)*s;
```

```
   }
   else //do continued fraction
   {
      for(k=n; k>=1; k--) c=k/(x+c);
      c=f(x)/(x+c);
      if(x>0) return 1.0-c; else return -c;
   }
}
```

Appendix C

C++ ptogram Regress.cpp

C++ Program Estimating $a^T\beta$ and σ^2.

```
\index{program!Regress.cpp}
//Regress.cpp
#include <stdio.h>
#include <iostream.h>
#include <fstream.h>
#include <stdlib.h>
#include <math.h>
#define sqr(x) ((x)*(x))
#define sign(x) (((x)<0)? -1 : 1)
#define abs(x) (((x)<0)? (-(x)):(x))
int n,p;
double *a,*Y,**X,*b,aTb,sigma2, Var_aTb, **S,**A;
void GetData(char *filename)
{
     int i,j;
     ifstream infile;
     infile.open(filename);
     if(!infile)
     {
          cout<<"Cannot open "<<filename<<" for input.\n";
          exit(1);
     }
     infile>>n>>p;
```

```
     a=new double[p+1];
     Y=new double[n+1];
     X=new (double*)[n+1];
     for(i=1; i<=n; i++) X[i]=new double[p+1];
     for(j=1; j<=p; j++) infile>>a[j];
     for(i=1; i<=n; i++)
     {
           infile>>Y[i];
           for(j=1; j<=p; j++) infile>>X[i][j];
     }
     infile.close();
}
void PrintData()
{
     int i,j;
     cout<<"\n\n(n,p)=("<<n<<", "<<p<<")\n\n";
     cout<<"(a";
     if(p==1) cout<<"[1])=";
     else if(p==2) cout<<"[1],a[2])=(";
            else cout<<"[1],...,a["<<p<<"])=(";
     for(j=1; j<p; j++) cout<<a[j]<<", ";
     cout<<a[p]<<")\n\n";
     cout<<"Y[i]: X[i,j] i=1,2,...,n, j=1,2,...,p. \n";
     cout<<"__________________________\n";
     for(i=1; i<=n; i++)
     {
          cout<<Y[i]<<"   : ";
          for(j=1; j<=p; j++) cout<<X[i][j]<<"  ";
          cout<<"\n";
     }
     cout<<"\n";
}
void XtoQR() //Householder method changes X=QR to R11,v1,v2,...,vp
{            // Q=Q1*Q2*...*Qp where Qi=I-2vi*vi'/(vi'*vi).
     int i,j1,j2;
     const double epsilon=1.0E-12;
     double norm, C, *v=new double[n+1], *w=new double[p+1];
     for(j1=1; j1<=p; j1++)
```

```
     {
          norm=0; //do house(X[j1:n,j1])
          for(i=j1; i<=n; i++) { norm+=sqr(X[i][j1]);  v[i]=X[i][j1]; }
          if(norm>epsilon)
          {
               norm=sqrt(norm);
               C=X[j1][j1]+sign(X[j1][j1])*norm;
               for(i=j1+1; i<=n; i++) v[i]/=C;
          }
          else { cout<<"Singular case, exit.\n"; exit(1); }
          v[j1]=1; //end of house(X[j1:n,j1])
          C=0;     //do row.house(X[j1:n, j1:p],v[j1:n])
          for(i=j1; i<=n; i++) C+=sqr(v[i]);
          C=-2.0/C;
          for(j2=j1; j2<=p; j2++)
          {
               w[j2]=0;
               for(i=j1; i<=n; i++) w[j2]+=X[i][j2]*v[i];
               w[j2]*=C;
          }
          for(i=j1; i<=n; i++)
               for(j2=j1; j2<=p; j2++) X[i][j2]+=v[i]*w[j2];
          for(i=j1+1; i<=n; i++) X[i][j1]=v[i];
    //end row.house(X[j1:n, j1:p),v[j1:n])
     }
     delete[ ] v;
     delete[ ] w;
}
// The matrix X[i,j] now has triangular R11 on or above the diagonal.
// The vector vj[j+1:n] is stored in column j below the diagonal, with
// vj[i]=0 for i<j and vj[j]=1 understood and not stored.
void YtoQTY()// Y is changed to Q'*Y=Qp*...*Q2*Q1*Y where
{            // Q1*Y=Y-C*v1,and C=2v1'*Y/(v1'*v1).
     int i,j;
     double C1,C2,C;
     for(j=1; j<=p; j++)
     {
          C1=Y[j]; C2=1; //since vj[i]=0 for i<j, and vj[j]=1,
```

```
          for(i=j+1; i<=n; i++) //we start at vj[j+1]... .
          {
               C1+=X[i][j]*Y[i];//get vj'*Y
               C2+=sqr(X[i][j]);//get vj'*vj
          }
          C=2.0*C1/C2;
          for(i=j; i<=n; i++)//get Y-C*vj
          {
               if(i==j) Y[i]-=C;
               else Y[i]-=C*X[i][j];
          }//Qj*...Q2*Q1*Y calculated
     }
}
void bSolve() // Solve R11*b=(Q'*Y)[1:p] for b, calculate a'*b, and S^2
{   // where a'*b=a[1]b[1]+...+a[p]b[p], S^2=(Y-Xb)'*(Y-Xb)/(n-p).
     int i,j;
     const double epsilon=1.0E-12;
     b=new double[p+1]; //regression coefficient space
     for(i=p; i>=1; i--)
          if(abs(X[i][i])>epsilon)
          {
               b[i]=Y[i];      //Y[1:p] stores (Q'*Y)[1:p]
               for(j=i+1; j<=p; j++) b[i]-=X[i][j]*b[j];
               b[i]/=X[i][i];  //X[i][j] stores R11[i][j], i<=j
          }                    //R11 is pxp upper triangular
          else { cout<<"Singular case.\n"; exit(1); }
     aTb=0;       for(i=1; i<=p; i++) aTb+=a[i]*b[i];
     sigma2=0;   for(i=p+1; i<=n; i++) sigma2+=sqr(Y[i]);
     sigma2/=(double)(n-p);
}
void GetVar() // Calculates estimate of Var(a'b)=a'(R11'R11)^{-1}a
{
     double *v=new double[p+1];
     int i,j;
     for(i=1; i<=p; i++)
     {
          v[i]=a[i];
          for(j=1; j<i; j++) v[i]-=X[j][i]*v[j];
```

```
          v[i]/=X[i][i];
     }
     Var_aTb=0;
     for(i=1; i<=p; i++) Var_aTb+=sqr(v[i]);
     Var_aTb*=sigma2;
     delete[ ] v;
}
void Cov()
{
     int i,j,k;
     S=new (double*)[p+1];//S for R11 inverse
     A=new (double*)[p+1];//A for R11^{-1}*R11^{-T}
     for(i=1; i<=p; i++)
     {
          S[i]=new double[p+1];
          A[i]=new double[p+1];
     }
     for(j=1; j<=p; j++)
          for(i=j; i>=1; i--)
          {
               if(i==j) S[i][i]=1;
               else S[i][j]=0;
               for(k=i+1; k<=j; k++) S[i][j]-=X[i][k]*S[k][j];
               S[i][j]/=X[i][i];
          }//S=Inverse(R11) calculated
     for(i=1; i<=p; i++)
          for(j=i; j<=p; j++)
          {
               A[i][j]=0;
               for(k=j; k<=p; k++) A[i][j]+=S[i][k]*S[j][k];
               A[i][j]*=sigma2;
          }//symmetric A=Cov(b) estimate calculated
     for(i=1; i<=p; i++)  for(j=1; j<i; j++) A[i][j]=A[j][i];
}//end of Cov( )
void PrintAnswers()
{
     int i,j;
     cout<<"b=(";
```

```
     for(i=1; i<p; i++) cout<<b[i]<<", ";
     cout<<b[p]<<")'\n\n";
     cout<<"Cov(b) estimate\n";
     for(i=1; i<=p; i++)
     {
          for(j=1; j<=p; j++)   cout<<setw(10)<<A[i][j]<<"  ";
          cout<<"\n";
     }
     cout<<"\n"<<"a'b= "<<aTb<<"\n\n";
     cout<<"S^2=(Y-Xb)'(Y-Xb)/(n-p)= "<<sigma2<<"\n\n";
}
void CleanUpData()
{
     int i;
     delete[ ] a;
     delete[ ] b;
     delete[ ] Y;
     for(int i=1; i<=n; i++) delete[ ] X[i];
     delete[ ] X;
     for(i=1; i<=p; i++){ delete[ ] S[i];  delete[ ] A[i]; }
     delete[ ] S; delete[ ] A;
}
int main(int argc, char *argv[ ])
{    // argv[1] is datafile name
     GetData(argv[1]);
     PrintData();
     XtoQR();
     YtoQTY();
     bSolve();
     GetVar();
     Cov();
     PrintAnswers();
     CleanUpData();
     return 0;
}
```

Appendix D

C++ program test.cpp for U.M.P. tests

The following C++ program calculates critical values and randomization constants for binomial, Poisson, or hypergeometric U.M.P. tests.

```
//Critical values program test.cpp.
//For binomial, hypergeometric, or Poisson.
#include <iostream.h>
#include "cdf.h" //(from chapter 3)
bool OK;
double n, p0, N, D0, lambda0, alpha, C=-1, xi;
char ch;
void getdata()
{
      do {
        cout<<"Enter b, h, or p for ";
        cout<<"binomial, hypergeometric, or Poisson:"; cin>>ch;
        OK=(ch=='b')||(ch=='h')||(ch=='p');
        if (!OK) cout<<"Error, enter again.\n"
      }while (!OK);
      if(ch=='b'){ cout<<"Enter n and p0 :"; cin>>n>>p0;}
      if(ch=='h'){ cout<<"Enter N, n, and D0 :"; cin>>N>>n>>D0;}
      if(ch=='p'){ cout<<"Enter lambda0 :"; cin>>lambda0;}
      cout<<"Enter alpha, 0<alpha<1 :"; cin>>alpha;
}
```

```
double F(double C)
{
      if(ch=='b') return cdf::icbeta(1.0-p0,n-C,C+1.0);
      if(ch=='h') return cdf::HyperG(C,N,D0,n);
      if(ch=='p') return 1.0-cdf::icgamma(lambda0,C+1.0);
}
void getCxi()
{
      double FC=0, FC1;
      do { FC1=FC; C++; FC=F(C);} while (FC<=(1.0-alpha));
      xi=(FC-(1.0-alpha))/(FC-FC1);
}
int main()
{
      getdata();
      getCxi();
      cout<<"(C,xi)=("<<C<<", "<<xi<<").\n";
      return 0;
}
```

Appendix E

C++ program Pvalue.cpp for some U.M.P.U. tests

```
//Pvalue.cpp
//UMPU test P-value program for the one sample binomial, Poisson,
//negative binomial, and the two sample binomial, Poisson,
//negative binomial distributions. Also the test.of independence
//for a 2x2 table with a multinomial(N,p11,p12,p21,p22) distribution
//Copyright (C) 2003 Jerome Klotz, Department of Statistics,
//University of Wisconsin, 1210 W. Dayton St.,Madison 53706.
#include <iostream.h>
#include <stdlib.h>
#include "cdf.h" //(from chapter 3)
double x,n,p0,lambda0, r;
double y,n1,n2,K0,s,r1,r2;
double N,x11,x12,x21,x22,x1p,xp1;
double L,U,L1,U1;
double c1,c2,gam1,gam2;
double m,alpha, epsilon=1.0e-10;
int k;
bool OK;

void PrintHeading(void)
{
   cout<<"P-value program for some discrete UMPU tests.\n\n";
}
```

```
void GetDist(void)
{
    char ch;
    do {
         cout<<"\nEnter an integer k where 0<=k<=7\n";
         cout<<"Enter 0 to exit\n";
         cout<<"One sample:  enter 1 binomial, 2 Poisson,";
         cout<<" 3 negative binomial\n";
         cout<<"Two samples: enter 4 binomial, 5 Poisson,";
         cout<<" 6 negative binomial\n";
         cout<<"Independence in a 2x2 table: enter 7 :"; cin>>ch;
         k=(int)(ch-'0'); //convert character to integer
         OK=(0<=k)&&(k<=7);
         if(!OK) cout<<"Incorrect entry. Please reenter:\n";
       }while(!OK);
    if(k==0) exit(0);
}
double F(double x)
{
    switch(k){
     case 1: if(x<-epsilon) return 0;
             if(x>(n-epsilon)) return 1;
             return cdf::icbeta(1-p0,n-x,x+1);
     case 2: if(x<-epsilon) return 0;
             return 1-cdf::icgamma(lambda0,x+1);
     case 3: if(x<-epsilon) return 0;
             return cdf::icbeta(p0,r,x+1);
     case 4: L=max(0,s-n2);  U=min(n1,s);
             if(x<(L-epsilon)) return 0;
             if(x>(U-epsilon)) return 1;
             return cdf::HyperG(x,n1+n2,s,n1);
     case 5: if (x<-epsilon) return 0;
             if(x>(s-epsilon)) return 1;
             return cdf::icbeta(1/(K0+1),s-x,x+1);
     case 6: if(x<-epsilon) return 0;
             return (1-cdf::HyperG(r1-1,r1+r2+s-1,r1+r2-1,r1+x));
     case 7: L=max(0,x1p+xp1-N); U=min(x1p,xp1);
             if(x<(L-epsilon)) return 0;
```

```
            if(x>(U-epsilon)) return 1;
            return cdf::HyperG(x,N,x1p,xp1); }
}
double F1(double x)
{
   switch(k){
     case 1: if(x<-epsilon) return 0;
             if(x>(n-1-epsilon)) return 1;
             return cdf::icbeta(1-p0,n-1-x,x+1);
     case 2: if(x<-epsilon) return 0;
             return 1-cdf::icgamma(lambda0,x+1);
     case 3: if(x<-epsilon) return 0;
             return cdf::icbeta(p0,r+1,x+1);
     case 4: L=max(0,s-1-n2); U=min(n1,s)-1;
             if(x<(L-epsilon)) return 0;
             if(x>(U-epsilon)) return 1;
             return cdf::HyperG(x,n1+n2-1,s-1,n1-1);
     case 5: if (x<-epsilon) return 0;
             if (x>(s-1-epsilon)) return 1;
             return cdf::icbeta(1/(K0+1),s-1-x,x+1);
     case 6: if(x<-epsilon) return 0;
             return (1-cdf::HyperG(r1,r1+r2+s-1,r1+r2,r1+1+x));
     case 7: L1=max(0,x1p+xp1-N-1); U1=min(x1p,xp1)-1;
             if(x<(L1-epsilon)) return 0;
             if(x>(U1-epsilon)) return 1;
             return cdf::HyperG(x,N-1,x1p-1,xp1-1); }
}
double f0(double x)
{
     return F(x)-F(x-1);
}
double f1(double x)
{
     return (F1(x)-F1(x-1));
}
void GetData(void)
{
     cout<<"\n";
```

```
 switch(k) {
  case 1:
   do {
         cout<<"One sample X:binomial(n,p) testing H:p=p0.\n";
         cout<<"Enter x n p0: "; cin>>x>>n>>p0;
         OK=(x>-epsilon)&&(x<(n+epsilon));
OK=OK&&(n>(1-epsilon))&&(p0>epsilon);
         if(!OK) cout<<"Incorrect entry. Reenter.\n";
       } while(!OK); break;
  case 2:
   do {
         cout<<"One sample X:Poisson(lambda"<<") ";
         cout<<"testing H:lambda =lambda0 .\n";
         cout<<"Enter x lambda0 :"; cin>>x>>lambda0;
         OK=(x>-epsilon)&&(lambda0>epsilon);
         if(!OK) cout<<"Incorrect entry. Reenter.\n";
       } while(!OK); break;
  case 3:
   do {
         cout<<"One sample X:negative binomial(r,p) ";
         cout<<"testing H:p=p0 .\n";
         cout<<"Enter x r p0 :"; cin>>x>>r>>p0;
         OK=(x>-epsilon)&&(r>epsilon)&&(p0>epsilon);
         if(!OK) cout<<"Incorrect entry. Reenter.\n";
       } while(!OK); break;
  case 4:
   do {
         cout<<"Two samples, independent X:binomial(n1,p1)";
         cout<<" and Y:binomial(n2,p2)\n";
         cout<<"testing H:p1=p2 .\n";
         cout<<"Enter x n1 y n2 :"; cin>>x>>n1>>y>>n2;
         OK=((x>-epsilon)&&(y>-epsilon));
         if(!OK) cout<<"Incorrect entry. Reenter.\n";
       } while(!OK); break;
  case 5:
   do {
         cout<<"Two samples, ";
         cout<<"independent X:Poisson(lambda1)";
```

```
            cout<<"and Y:Poisson(lambda2),\n";
            cout<<"testing H: lambda1=K*lambda2 .\n";
            cout<<"Enter x y K :"; cin>>x>>y>>K0;
            OK=((x>-epsilon)&&(y>-epsilon)&&(K0>epsilon));
            if(!OK) cout<<"Incorrect entry. Reenter.\n";
          } while(!OK); break;
      case 6:
       do {
            cout<<"Two samples, independent X:negative ";
    cout<<"binomial(r1,p1) and\n";
            cout<<"Y:negative binomial(r2,p2) testing H:p1=p2 .\n";
            cout<<"Enter x r1 y r2 :"; cin>>x>>r1>>y>>r2;
            OK=((x>-epsilon)&&(y>-epsilon));
            OK=OK&&((r1>(1-epsilon))&&(r2>(1-epsilon)));
            if(!OK) cout<<"Incorrect entry. Reenter.\n";
          } while(!OK); break;
      case 7:
       do {
            cout<<"Test of independence in a 2x2 table.\n";
            cout<<"X=(X11,X12,X21,X22):multinomial";
    cout<<"(N, p[1,1],p[1,2],p[2,1],p[2,2])\n";
            cout<<"testing H:p[i,j]=p[i,+]*p[+,j] for all i,j=1,2\n";
            cout<<"where p[i,+]=p[i,1]+p[i,2], p[+,j]=p[1,j]+p[2,j].\n";
            cout<<"Enter x11 x12 :"; cin>>x11>>x12;
            cout<<"Enter x21 x22 :"; cin>>x21>>x22;
            OK=(x11>-epsilon)&&(x12>-epsilon);
    OK=OK&&(x21>-epsilon)&&(x22>-epsilon);
            if(!OK) cout<<"Incorrect entry. Reenter.\n";
          } while(!OK); break;}
} //end GetData
void SetParameters(void)
{
    switch(k) {
     case 1: case 2: case 3:  break;
     case 4: s=x+y;  N=n1+n2; break;
     case 5: case 6: s=x+y;   break;
     case 7: x=x11; x1p=x11+x12; xp1=x11+x21;
             N=x11+x12+x21+x22; break; }
```

```
}
double mode()
{
    switch(k) {
     case 1: return floor((n+1)*p0+epsilon);
     case 2: return floor(lambda0+epsilon);
     case 3: return floor((r-1)*(1-p0)/p0+epsilon);
     case 4: return floor((n1+1)*(s+1)/(N+2)+epsilon);
     case 5: return floor((s+1)*K0/(1+K0)+epsilon);
     case 6: if(abs(r1+r2-1)<epsilon) return 0;
             return floor((r1-1)*(s+1)/(r1+r2-2)+epsilon);
     case 7: return floor((x1p+1)*(xp1+1)/(N+2)+epsilon); }
}
double LowerValue(void)
{
    switch(k) {
     case 1: case 2: case 3: case 5: case 6: return 0;
     case 4: return max(0,s-n2);
     case 7: return max(0,x1p+xp1-N); }
}
double UpperValue(void)
{
    switch(k) {
     case 1: return n;
     case 2: case 3: return 3*mode();
     case 4: return min(n1,s);
     case 5: case 6: return s;
     case 7: return min(x1p,xp1);}
}
void GetPval(void)
{
      bool OK,LowerTail;
      double gam1bar,gam2bar;
      m=mode();
      if(abs(x-m)<epsilon)
      {
          cout<<"x=mode="<<m<<" .\n"; alpha=1;
          if(m<(UpperValue()-epsilon))
```

```
            { c1=m; gam1=1; c2=m+1; gam2=1;}
            else { c2=m; gam2=1; c1=m-1; gam1=1;}
        }
        else
        {
            LowerTail=(x<(m+epsilon));
            if(LowerTail)
            {
                cout<<"Lower tail.\n";
                gam1=1; c1=x; c2=UpperValue();
                do {
                     gam2bar=(F1(c2-2)-F1(c1-1)-(F(c2-1)-F(c1)))/(f0(c2)-f1(c2-1));
                     OK=(gam2bar<(1+epsilon))&&(gam2bar>=-epsilon);
                     if(!OK) c2--;
                     if(c2<(x+epsilon)) {cout<<"No convergence.\n"; exit(0);}
                   }while(!OK);
                gam2=1-gam2bar;
            }
            else //upper tail
            {
                cout<<"Upper tail.\n";
                gam2=1; c2=x; c1=LowerValue();
                do {
                     gam1bar=(F1(c2-2)-F1(c1-1)-F(c2-1)+F(c1))/(f0(c1)-f1(c1-1));
                     OK=(gam1bar<(1+epsilon))&&(gam1bar>-epsilon);
                     if(!OK) c1++;
                     if(c1>(x-epsilon)) {cout<<"No convergence.\n"; exit(0);}
                   }while(!OK);
                gam1=1-gam1bar;
            }
            if(abs(gam1)<epsilon) gam1=0;//round to zero
            if(abs(gam2)<epsilon) gam2=0;
            alpha=F(c1-1)+gam1*f0(c1)+gam2*f0(c2)+1-F(c2);
        }
} //end GetPval
void PrintData(void)
{
   switch(k){
```

```
   case 1: cout<<"(x,n,p0)=("<<x<<", "<<n<<", "<<p0<<").\n"; break;
   case 2: cout<<"(x,lambda0)=("<<x<<", "<<lambda0<<").\n";  break;
   case 3: cout<<"(x,r,p0)=("<<x<<", "<<r<<", "<<p0<<").\n"; break;
   case 4: cout<<"(x,n1)=("<<x<<", "<<n1<<"),";
           cout<<" (y,n2)=("<<y<<", "<<n2<<").\n"; break;
   case 5: cout<<"(x,y)=("<<x<<", "<<y<<"), K="<<K0<<" .\n"; break;
   case 6: cout<<"(x,r1)=("<<x<<", "<<r1<<"),";
           cout<<"(y,r2)=("<<y<<", "<<r2<<").\n"; break;
   case 7: cout<<"(x11,x12,x21,x22)=("<<x11<<", "<<x12<<", ";
           cout<<x21<<", "<<x22<<").\n"; break; }
}
void PrintAns(void)
{
   cout<<"Pvalue("<<x<<")= "<<alpha<<"\n";
   cout<<"Critical values (C1,C2)=("<<c1<<", "<<c2<<").\n";
   cout<<"Randomization probabilities (gamma1,gamma2)=(";
   cout<<gam1<<", "<<gam2<<"). \n";
}
int main()
{
    PrintHeading();
    do {
         GetDist();
         GetData();
         SetParameters();
         GetPval();
         PrintData();
         PrintAns();
       }while(true);
    return 1;
}
```

Appendix F

C++ program rxcIndep.cpp testing independence

The following C++ program calculates the exact P-value for the conditional likelihood ratio test of independence in an rxc contingency table for small cases.

```
//rxcIndep.cpp
#include <iostream.h>
#include <fstream.h>
#include <math.h>
#define min(x,y) (((x)<(y))? (x):(y))
int r,c,i,j;
const double epsilon=1.0e-10;
int **X, *Xrow, *Xcol, **U, *Urow, *Ucol, n;
long MatrixCount;
double m2lnLam; //-2ln(lambda)
double Pval;
double s0; //constant parts of prob

void PrintHeading(void)
{
 cout<<"Likelihood ratio test conditional on the ";
 cout<<"margins X[i,+],X[+,j]\n";
 cout<<"for an rxc table X[i,j] i=1,2,...,r, ";
 cout<<"j=1,2,...,c with multinomial\n";
```

```
 cout<<"dist. testing independence H: p[i,j]=p[i,+]p[+,j]";
 cout<<" for all i,j.\n\n";
 cout<<"The program generates all non negative integer ";
 cout<<"component matrices u \n";
 cout<<"with margins equal to X[i,+],X[+,j]. ";
 cout<<"The P-value is computed by adding\n";
 cout<<"up P(u|X[i,+],X[+,j]) for each matrix u with ";
 cout<<"T(u)>=T(X) where X is \n";
 cout<<"the data matrix & T is equivalent to the LR";
 cout<<"statistic -2ln(lambda).\n\n";
}//end PrintHeading
void GetData(char *filename)
{
 ifstream infile;
 infile.open(filename);
 if(!infile){ cout<<"Cannot open "<<filename<<" for input.\n"; exit(1);}
 infile>>r>>c;
 X=new (int*)[r+1];
 for(i=1; i<=r; i++) X[i]=new int[c+1];
 for(i=1; i<=r; i++) for(j=1; j<=c; j++) infile>>X[i][j];
 infile.close();
}//end GetData
void SetUMatrix(void)
{
 U=new (int*)[r+1];
 for(i=1; i<=r; i++) U[i]=new int[c+1];
 Urow=new int[r+1];  Ucol=new int[c+1];
}//end SetUMatrix
void SetMargins(void) //sets row, col margins and n
{
 Xrow=new int[r+1]; Xcol=new int[c+1];
 for(i=1; i<=r; i++)
 {
  Xrow[i]=0;
  for(j=1; j<=c; j++)  Xrow[i]+=X[i][j];
   if(Xrow[i]==0) { cout<<"Zero row margin, exit.\n"; exit(0);}
 }
 for(j=1; j<=c; j++)
```

```
 {
  Xcol[j]=0;
  for(i=1; i<=r; i++) Xcol[j]+=X[i][j];
   if(Xcol[j]==0) { cout<<"Zero column margin, exit.\n"; exit(0);}
 }
 n=0; for(i=1; i<=r; i++) n+=Xrow[i];
}//end SetMargins
void PrintCounts(int **x, char *name)
{
 cout<<"\n"<<name;
 for(i=1; i<=r; i++)
 {
  cout<<"\n| ";
  for(j=1; j<=c; j++){ cout.width(4); cout<<x[i][j]<<" ";}
  cout<<" |"<<Xrow[i];
 }
 cout<<"\n|_";
 for(j=1; j<=c; j++) cout<<"_____";
 cout<<"_|\n  ";
 for(j=1; j<=c; j++) { cout.width(4); cout<<Xcol[j]<<" ";}
 cout<<" |"<<n<<"\n";
}//end PrintCounts
double lnfac(int n)
{ //log(n!) by Stirling's formula and Binet cont. frac.error funct.
 if (n<2) return 0.0;
 double r, dn=n, lnsq2pi=0.918938533204673; // 0.5*log(2*pi)
  double a1=1.0/12.0, a2=1.0/30.0, a3=53.0/210.0, a4=195.0/371.0;
 double a5=22999.0/22737.0, a6=29944523.0/19733142.0;
 double a7=109535241009.0/48264275462.0;
 r=dn+a7/dn; r=dn+a6/r; r=dn+a5/r; r=dn+a4/r;  r=dn+a3/r; r=dn+a2/r;
 return (lnsq2pi-dn +(dn+0.5)*log(dn)+a1/r);
}//end lnfac
void InitProb(void)
{
 s0=-lnfac(n);
  for(i=1; i<=r; i++) s0+=lnfac(Xrow[i]);
  for(j=1; j<=c; j++) s0+=lnfac(Xcol[j]);
}//end InitProb
```

```
double Prob(void)
{
 double s=s0; //constant terms from InitProb
 for(i=1; i<=r; i++)
  for(j=1; j<=c; j++) s-=lnfac(U[i][j]);
 return exp(s);
}//end Prob
double LRStat(int **x)
{
 double stat=0;
 for(i=1; i<=r; i++)
  for(j=1; j<=c; j++)
   if(x[i][j]>0)
    stat+=x[i][j]*log((double)(x[i][j]*n)/(double)(Xrow[i]*Xcol[j]));
 return 2*stat;
}//end LRStat
double T(int **x) //equivalent statistic
{
 double stat=0;
 for(i=1; i<=r; i++) for(j=1; j<=c; j++)
   if(x[i][j]>0) stat+=x[i][j]*log(x[i][j]);
 return stat;
}//end T
void LexOrd(int i1)
{     //rows i1,i1+1,...,r of U set to "smallest" order
 for(j=1; j<=c; j++) Ucol[j]=Xcol[j];
 for(i=1; i<=r; i++) Urow[i]=Xrow[i];
 if(i1>1) for(j=1; j<=c; j++) for(i=1; i<i1; i++) Ucol[j]-=U[i][j];
 for(i=i1; i<=r; i++) for(j=1; j<=c; j++)
  {
   U[i][j]=min(Urow[i],Ucol[j]);
   Urow[i]-=U[i][j]; Ucol[j]-=U[i][j];
  }
}//end LexOrd
bool ChangeRow(int i1) //changes the i1-th row of U to the next largest
{ //then resets rows i1+1,...,r & returns true else returns false at end.
 int j0, s;
 bool cellfull;
```

```
 for(j=1; j<=c; j++) Ucol[j]=Xcol[j];
 if(i1>1) for(j=1; j<=c; j++) for(i=1; i<i1; i++) Ucol[j]-=U[i][j];
 s=-1; j=0;
 do j++; while (U[i1][j]==0);
 if(j==c) return false;
 else
 {
   do
   {
     s+=U[i1][j]; j++;
     cellfull=(U[i1][j]==min(Xrow[i1],Ucol[j]));
   } while (cellfull&&(j<c));
   if(cellfull) return false;
   else //modify row
   {
     U[i1][j]++; j0=j-1;
     for(j=1; j<=j0; j++){ U[i1][j]=min(s,Ucol[j]); s-=U[i1][j];}
     return true;
   }
 }
}//end ChangeRow
bool Next(void) // returns true if U modified to next largest,
{               // otherwise returns false at end.
 bool done;
 int i1=r;
 do { i1--; done=ChangeRow(i1);} while((!done)&&(i1>1));
 if(done) LexOrd(i1+1);
 return done;
}//end Next
void PrintTestStat(void)
{
 m2lnLam=LRStat(X);
 cout<<"-2ln(lambda)="<<m2lnLam<<"\n";
}//end PrintTestStat
void SetPval(void)
{
 MatrixCount=0; Pval=0;
 LexOrd(1); //sets starting matrix U
```

```
 PrintCounts(U,"Starting Matrix"); //smallest in lexical order
 InitProb(); //set constants in probabilities
 double T0=T(X); //T0 is equivalent statistic for data X
 do { MatrixCount++; if(T(U)>(T0-epsilon)) Pval+=Prob(); } while(Next());
 //Next() changes U matrix to next largest in lexical order
 PrintCounts(U,"Ending Matrix"); //largest in lexical order
}//end SetPval
void PrintAnswers(void)
{
 cout<<"\nP-value:\n";
 cout<<"P[-2ln(lambda)>="<<m2lnLam<<"|X[i,+],X[+,j]]="<<Pval<<"\n";
 cout<<"\nTotal matrices enumerated="<<MatrixCount<<".\n";
}//end PrintAnswers
void DeleteArrays(void)
{
 for(i=1; i<=r; i++) { delete[] X[i];delete[] U[i];}
 delete[] X; delete[] Xrow; delete[] Xcol;
 delete[] U; delete[] Urow; delete[] Ucol;
}//end DeleteArrays

int main(int argc, char* argv[])
{ //argv[] is name of file with r, c, and X[i,j] values
 PrintHeading();
 GetData(argv[1]);
 SetUMatrix();
 SetMargins();
 PrintCounts(X,"Data Matrix X");
 PrintTestStat();
 SetPval();
 PrintAnswers();
 DeleteArrays();
 return 1;
}
```

Appendix G

C++ program OneVar.cpp for the confidence interval for σ^2

The following C++ program gives the unbiased confidence interval for the variance using a sample from a normal distribution.

```
//OneVar.cpp Unbiased confidence interval program for a normal variance.
#include <stdlib.h>
#include <iostream.h>
#include <math.h>
#include "cdf.h"                // see chapter 3 page 60
const double epsilon=1.0e-10;   // equation tolerance for integral
double df;                      // degrees of freedom nu=n-1 or n
double U;                       // chi square value
double rLower, rUpper, r;       // r=C1/C2
double C1, C2;                  // critical values
double d1, d2, alphabar;        // integrals, 1-alpha
double LowerBound, UpperBound; // bounds for sigma^2

double F(double m, double u)    // F(m,u)=P[U<u], U is chi-square m=df.
{                               // Incomplete gamma is used.
        return cdf::icgamma(u/2.0,m/2.0);
}
void GetData(void)
{
        cout<<"Enter integer degrees of freedom df>0: ";
```

```
        cin>>df;
        cout<<"Enter chi square value U>0: ";
        cin>>U;
        cout<<"Enter confidence coefficient 0<1-alpha<1: ";
        cin>>alphabar;
        if((df<1)||(U<0)||(alphabar<epsilon)||(alphabar>(1.0-epsilon)))
        {
                cout<<"Invalid data, (df,U,1-alpha)="<<df<<", ";
                cout<<U<<", "<<alphabar<<") exit.\n"; exit(0);
        }
}
void GetC1C2(void)
{
        rLower=0; rUpper=1.0;
        do {
                r=(rLower+rUpper)/2.0;
                C2=df*log(r)/(r-1);
                C1=r*C2;
                d1=F(df,C2)-F(df,C1);
                if(d1<alphabar) rUpper=r;
                else if(d1>alphabar) rLower=r;
           } while(fabs(d1-alphabar)>epsilon);
}
void PrintAnswers(void)
{
  cout<<"r=C1/C2= "<<r<<"\n";
  d2=F(df+2.0,C2)-F(df+2.0,C1); LowerBound=U/C2; UpperBound=U/C1;
  cout<<"(C1, C2)=("<<C1<<", "<<C2<<")\n";
  cout<<"F("<<df<<","<<C2<<")-F("<<df<<","<<C1<<")="<<d1<<"\n";
  cout<<"F("<<df+2.0<<","<<C2<<")-F("<<df+2.0<<","<<C1<<")="<<d2<<"\n";
  cout<<"The "<<100.0*alphabar<<" percent confidence interval for the";
  cout<<" variance is ("<<LowerBound<<", "<<UpperBound<<").\n";
}
int main(void)
{
        GetData();
        GetC1C2();
        PrintAnswers();
```

```
        return 1;
}
```

Appendix H

C++ program for the unbiased confidence interval for σ^2/τ^2

The following C++ program calculates the confidence interval for the ratio of two variances given the degrees of freedom and the sums of squares from two normal samples.

```
//TwoVar.cpp program to calculate the confidence interval for the
//ratio of two variances of samples from two normal distributions.
#include <iostream.h>
#include <math.h>
#include <stdlib.h>
#include "cdf.h" //see chapter 3 page 60

double alphabar;
double df1, df2;// degrees of freedom (m-1,n-1) or (m,n)
double Sx2, Sy2;
// sums of squares (sum(Xi-ave(X))^2, sum(Yj-ave(Y))^2)
double C1, C2, C1Lower, C1Upper, C2Lower, C2Upper;
//beta critical values, bounds
double d1, d2, e1, e2; //integral values, values of h function
const double epsilon=1.0e-10; //tolerance for convergence

double h(double x)
{
   return df1*log(x)+df2*log(1.0-x);
```

```
}
void GetData(void)
{
   bool bad;
   cout<<"Unbiased confidence interval for the ratio of ";
   cout<<two variances.\n\n";
   cout<<"Enter confidence coefficient 1-alpha: ";
   cin>>alphabar;
   cout<<"Enter degrees of freedom df1 and df2: ";
   cin>>df1>>df2;
   cout<<"Enter sums of squares Sx2 and Sy2: ";
   cin>>Sx2>>Sy2;
   bad=(alphabar<epsilon)||(alphabar>(1-epsilon));
   bad=bad||(df1<1)||(df2<1)||(Sx2<epsilon)||(Sy2<epsilon);
   if(bad)
   {
     cout<<"Invalid data (1-alpha, df1, df2, Sx2, Sy2)=("<<alphabar;
     cout<<", "<<df1<<", "<<df2<<", "<<Sx2<<", "<<Sy2<<"), exit.\n";
     exit(0);
   }
}
void GetC1C2(void)
{
   double bound=df1/(df1+df2);
   C1Lower=0; C1Upper=bound;
   do
   {
      C1=(C1Lower+C1Upper)/2.0;
      e1=h(C1);
      C2Lower=bound; C2Upper=1.0;
      do
      {
         C2=(C2Lower+C2Upper)/2.0;
         e2=h(C2);
         if(e2>e1) C2Lower=C2;
         else if(e2<e1) C2Upper=C2;
      } while(fabs(e2-e1)>epsilon);
      d1=cdf::icbeta(C2,df1/2.0,df2/2.0)-cdf::icbeta(C1,df1/2.0,df2/2.0);
```

```
      if(d1<alphabar) C1Upper=C1;
      else if(d1>alphabar) C1Lower=C1;
   } while(fabs(d1-alphabar)>epsilon);
   d2=cdf::icbeta(C2,(df1+2.0)/2.0,df2/2.0)-cdf::icbeta(C1,(df1+2.0)/2.0,df2/2.0);
}
void PrintAnswers(void)
{
   double r=df1/df2, x1=C1/(r*(1-C1)), x2=C2/(r*(1-C2)), x=Sx2/(r*Sy2);
   cout<<"\nBeta dist. critical values: (C1,C2)=("<<C1<<","<<C2<<").\n";
   cout<<"I("<<C2<<", "<<df1/2.0<<", "<<df2/2.0<<")-I("<<C1<<", ";
   cout<<df1/2.0<<", "<<df2/2.0<<")="<<d1<<" .\n";
   cout<<"I("<<C2<<", "<<(df1+2.0)/2.0<<", "<<df2/2.0<<")-I("<<C1;
   cout<<", "<<(df1+2.0)/2.0<<", "<<df2/2.0<<")="<<d2<<" .\n";
   cout<<"F ratio (Sx2/df1)/(Sy2/df2)="<<x<<" .\n";
   cout<<"F distribution critical values: (F1,F2)=("<<x1<<", "<<x2<<").\n";
   cout<<"The variance ratio "<<100*alphabar<<" percent confidence ";
   cout<<"interval value is ("<<x/x2<<", "<<x/x1<<").\n\n";
}
int main(void)
{
   GetData();
   GetC1C2();
   PrintAnswers();
   return 1;
}
```

Appendix I

C++ program for unbalanced multiway ANOVA

The following C++ program, **multiway.cpp**, calculates an ANOVA table.

```
//multiway.cpp a program for multifactor analysis of variance.
//Copyright (C) 2003, Jerome H. Klotz. University of Wisconsin.
#include <stdlib.h>
#include <iostream>
#include <fstream>
#include <iomanip>
#include <cmath>
#include <list>
#include <iterator>
#include "cdf.h"
using namespace std;

const int nmax=50;//maximum cell count
int M, N, p;    // cell count, total observations, # factors
int *L, *n;     // L[i]=levels i-th factor, n[j] # in cell j
double **Y;     // data Y[i][j],0<i<=M, 0<j<=n[i]
double *Ybar;   // Ybar[i]=Y[i][*] weighted averages
double **w;     // w[i][j] are weights
double **A,*b;  // A ,b are for solving for lambda
double *lambda; // lambda- LaGrange multiplier values
int *nu;        // nu[k]=size k-th block of b
```

```
int *NuSum;     // NuSum[i]=nu[1]+...+nu[i]
int Nu;         // Nu=sum nu[i]: for i=1,2,...k
list<int> Dp;   // Dp=(1, L[1], L{1]*L[2],..., L[1]*L[2]*..*.L[p])
list<int> Hp;   // Hp=(1, 2,..., p)

void GetData(char *filename)
{
     int i,j;
     char ch;
     double buffer[nmax+1];
     ifstream infile;
     infile.open(filename);
     if(!infile)
     {
        cout<<"Cannot open "<<filename<<" for input.\n";
        exit(1);
     }
     infile>>p;
     if(p<1)
     {
        cout<<"Number of factors is less than 1, exit.\n";
        exit(1);
     }
     L=new int[p+1];
     for(i=1; i<=p; i++)
     {
        infile>>L[i];
        if(L[i]<2)
        {
           cout<<"There exists a level less than 2, exit.\n";
           exit(1);
        }
     }
     do ch=infile.get(); while(!isdigit(ch));//move to next line
     infile.putback(ch);
     M=L[1];
     for(i=2; i<=p; i++) M*=L[i];
     n=new int[M+1];
```

```
     Y=new (double*)[M+1];
     for(i=1; i<=M; i++)
     {
        n[i]=0;
        while((ch=infile.get())!='\n')
        {
           if(isdigit(ch))
           {
               infile.putback(ch);
               n[i]++;
               infile>>buffer[n[i]];
           }
        }
        Y[i]=new double[n[i]+1];
        for(j=1; j<=n[i]; j++) Y[i][j]=buffer[j];
    }
}
void SetWeights(void)
{
     int i,j;
     double sum;
     char ch;
     w=new (double*)[p+1];
     for(i=1; i<=p; i++) w[i]=new double[L[i]+1];
     cout<<"Do you want equal weights? Enter Y)es or N)o :";
     cin>>ch;
     if((ch=='y')||(ch=='Y'))
       for(i=1; i<=p; i++) for(j=1; j<=L[i]; j++) w[i][j]=1.0/L[i];
       else
       {
         cout<<"Enter weights w[i][j] for i=1,...,"<<p;
 cout<<", j=1,...,L[i]\n";
         for(i=1; i<=p; i++)
         {
            cout<<"i="<<i<<" Enter "<<L[i];
            cout<<" weights that add to 1.0 :\n";
            for(j=1; j<=L[i]; j++)
            {
```

```
              cout<<"w["<<i<<"]["<<j<<"]=";
              cin>>w[i][j];
           }
        }
        for(i=1; i<=p; i++)//make weights add to one.
        {
           sum=0;
           for(j=1; j<=L[i]; j++) sum+=w[i][j];
           if(sum>0) for(j=1; j<=L[i]; j++) w[i][j]/=sum;
           else // if zero, exit
           {
              cout<<"Zero weights, exit. \n";
              exit(1);
           }
        }
      }
}
void SetYbar_N(void)
{
     int i,j;
     N=0;
     for(i=1; i<=M; i++) N+=n[i];
     Ybar=new double[M+1];
     for(i=1; i<=M; i++)
     {
        Ybar[i]=0;
        for(j=1; j<=n[i]; j++) Ybar[i]+=Y[i][j];
        Ybar[i]/=(double)n[i];
     }
}
void SetDD(list<int> &DD, int s, list<int> hh)
{ //for address calculation
     int j,K;
     list<int>::iterator is,it;
     DD.erase(DD.begin(),DD.end());
     if(s!=0)
     {
        is=hh.begin(); advance(is,s-1);
```

```
        hh.erase(is);
     }
     is=hh.begin();
     K=hh.size();
     DD.push_back(1);
     it=DD.begin();
     for(j=1; j<K; j++)
     {
        if(j<s) DD.push_back((L[(*is)]-1)*(*it));
        else  DD.push_back(L[(*is)]*(*it));
        is++; it++;
     }
}
void SetStorage(void)//M=L[1]*L[2]*...*L[p]>Nu
{
     int i;
     nu=new int[p+1];
     NuSum=new int[p+1];
     A=new (double*)[M+1];//triangular storage A[i,j]=A[j,i]
     for(int i=1; i<=M; i++) A[i]=new double[i+1];
     b=new double[M+1];
     lambda=new double[M+1];
     Hp.erase(Hp.begin(),Hp.end());
     for(i=1; i<=p; i++) Hp.push_back(i);
     SetDD(Dp,0,Hp);
}
int Address(list<int> ii, list<int> DD)
{//sets address from list ii using DD
     int j=0;
     list<int> ::iterator s,t;
     t=DD.begin();
     for(s=ii.begin(); s!=ii.end(); s++)
     {
        j+=((*s)-1)*(*t);
        t++;
     }
     return ++j;
}
```

```
void Initialize(list<int> &hh)
{// sets starting list (1)
     hh.erase(hh.begin(),hh.end());
     hh.push_back(1);
}
bool Change(list<int> &hh)//changes list hh to next largest in
{// lexical order. Returns true if possible, otherwise false.
     int k=hh.size(),k2=0,j,r,pmax=p;
     if(k==p) return false; //no modification
     list<int> ::reverse_iterator ri;
     list<int> ::iterator fi1,fi2 ;
     ri=hh.rbegin();
     while(((*ri)==pmax)&&(ri!=--hh.rend()))
     {
        pmax--; ri++;
     }
     if((*ri)!=pmax) //increment value < pmax and reset
     {
        r=(*ri);
        fi2=find(hh.begin(),hh.end(),r);
        for(fi1=fi2; fi1!=hh.end(); fi1++) k2++;
        hh.erase(fi2,hh.end());
        for(j=r+1; j<=(r+k2); j++) hh.push_back(j);
     }
     else //set beginning subset with one more element
     {
        hh.erase(hh.begin(),hh.end());
        for(j=1; j<=k+1; j++) hh.push_back(j);
     }
     return true;
}
void PrintList(list<int> LL, char ch)
{ //prints list LL followed by a character
     list<int>::iterator fi;
     cout<<"(";
     if(LL.empty()) cout<<")"<<ch;
     else
      for(fi=LL.begin(); fi!=LL.end(); fi++)
```

```
        cout<<*fi<<( (fi==(--LL.end())) ? ")":",");
     cout<<ch;
}
void SetComplement(list<int> &hc, list<int> hh )
{ // sets complement list hc=hp -hh
     int j;
     list<int>::iterator s;
     hc.erase(hc.begin(), hc.end());
     for(j=1; j<=p; j++)
     {
        s=find(hh.begin(),hh.end(),j);
        if(s==hh.end()) hc.push_back(j);
     }
}
void SetList(list<int> &ii, int j, int s, list<int> hh)
//sets list (i1,i2,...,ik)<--> j using hh and block s
{
     list<int> DD;
     list<int>::reverse_iterator ri;
     list<int>::iterator it;
     ii.erase(ii.begin(),ii.end());
     if((hh.size()>1)||(s==0))
     {
        SetDD(DD,s,hh);
        int R=j-1; //cout<<"R="<<R<<"\n";
        for(ri=DD.rbegin(); ri!=DD.rend(); ri++)
        {
           ii.push_front(R/(*ri));
           it=ii.begin();
           R-=(*it)*(*ri);
        }
        for(it=ii.begin(); it!=ii.end(); it++) (*it)++;
     }
}
void PrintData(void)
{
     int j,k;
     list<int> ii;
```

```
     char ch;
     cout<<"Do you want to print out the data? Enter Y)es or N)o :";
     cin>>ch;
     if((ch=='y')||(ch=='Y'))
     {
        cout<<"\nData:-a total of "<<N<<" observations. ";
        cout<<p<<((p==1)?" factor":" factors")<<" with ";
        if(p==1) cout<<L[1]<<" levels.\n";
        else
        {
           cout<<"levels (";
           for(j=1; j<=p; j++) cout<<L[j]<<((j==p)?").\n":", ");
        }
        cout<<"  j  cell";
        cout<<setfill(' ')<<setw(2*p)<<" ";
        cout<<"n(j)   Y.[j]    |  Y[j][k] for k=1,2,...,n[j] \n";
        cout<<setfill('_')<<setw(3*p+56)<<"_"<<"\n";
        for(j=1; j<=M; j++)
        {
           cout<<setfill(' ')<<setw(3)<<j<<"  ";
           SetList(ii,j,0,Hp);
           PrintList(ii,' ');
           cout<<setw(4)<<n[j]<<"   ";
           cout<<fixed<<setw(9)<<setprecision(4)<<Ybar[j]<<"  |   ";
           for(k=1; k<=n[j]; k++)
           cout<<fixed<<setw(9)<<setprecision(4)<<Y[j][k]<<"  ";
           cout<<"\n";
        }
     }
}
void InitializeList(list<int> &ii, list<int> hh)
{//sets starting list ii=(1,1,...,1) from hh=(h1,h2,...,hk)
     int j,k=hh.size();
     ii.erase(ii.begin(),ii.end());
     for(j=1; j<=k; j++) ii.push_back(1);
}
bool IncrementList(list<int> &ii, list<int> hh)
{ //increments (i1,i2,...,ik) if possible
```

```
     int j,k1=0;
     list<int>::iterator t1,t2,t3;
     t3=hh.begin();
     for(t1=ii.begin(); t1!=ii.end(); t1++)
       if((*t1)<L[(*t3)])
       {
          (*t1)++;
          for(t2=ii.begin(); t2!=t1; t2++) k1++;
          ii.erase(ii.begin(), t1);
          for(j=1; j<=k1; j++) ii.push_front(1);
          return true;
       }
       else  t3++;
       return false;
}
void Merge(list<int> ii, list<int> ic, list<int> &ip, list<int> hh)
{// puts lists ii and ic together to form list ip
     int j;
     list<int>::iterator sii, sic;
     ip.erase(ip.begin(),ip.end());
     sii=ii.begin(); sic=ic.begin();
     for(j=1; j<=p; j++)
       if(find(hh.begin(),hh.end(),j)==hh.end())
       {
          ip.push_back((*sic)); sic++;
       }
       else
       {
          ip.push_back((*sii)); sii++;
       }
}
double V(list<int> hh, int j)
{
     int i,jj;
     double v=0, WW=1.0;
     list<int>  LL,Lc,DD,Dc,hc,ii,ic,ip;
     list<int>::iterator itic,itHc;
     SetComplement(hc,hh); //hc set
```

```
     SetList(ii,j,0,hh);
     if(!hc.empty())
     {
        InitializeList(ic,hc);
        do
        {
           Merge(ii,ic,ip,hh);
           jj=Address(ip,Dp);
           WW=1.0;
           itHc=hc.begin();
           for(itic=ic.begin(); itic!=ic.end(); itic++)
           {
              WW*=sqr(w[(*itHc)][(*itic)]);//sqr(x)=x*x
              itHc++;
           }
           v+=WW/n[jj];
        }while(IncrementList(ic,hc));
        return 1.0/v;
     }
    else  return n[j]; //case hh=(1,2,...p)
}
void SetNus(list<int> hh)
{
     int k,s,t,K=hh.size();
     list<int>:: iterator it;
     for(k=1; k<=K; k++)
     {
        nu[k]=1; it=hh.begin();
        for(s=1;s<k; s++)
        {
           nu[k]*=(L[(*it)]-1); it++;
        }
        it++;
        for(t=(k+1); t<=K; t++)
        {
           nu[k]*=L[(*it)]; it++;
        }
     }
```

```
     NuSum[0]=0;
     for(k=1; k<=K; k++) NuSum[k]=NuSum[k-1]+nu[k];
}
void SetBlockIndices(int j, int &kk, int &jj)
{  // kk is block, jj is index in block
     kk=1;
     while (j>NuSum[kk]) kk++;
     jj=j-NuSum[kk-1];
}
double Ybar_dot(list<int> hh, int j)
{
     int i,jj;
     double Y_dot=0, WW; //WW is product of weights for hc
     list<int>  ic,ii,ip,hc;
     list<int>::iterator it,is;
     SetList(ii,j,0,hh);
     SetComplement(hc,hh); //hc set
     InitializeList(ic,hc);
     do
     {
        Merge(ii,ic,ip,hh);
        jj=Address(ip,Dp);
        WW=1.0; it=ic.begin();
        for(is=hc.begin(); is!=hc.end(); is++)
        {
           WW*=w[(*is)][(*it)]; it++;
        }
        Y_dot+=Ybar[jj]*WW;
     }while(IncrementList(ic,hc));
     return Y_dot;
}
bool Compatible(list<int> iis1,list<int> iis2,int s1, int s2)
{
     bool same=true;
     int i,r=min(s1,s2),s=max(s1,s2),K=iis1.size()+1;
     list<int>::iterator it1,it2;
     it1=iis1.begin(); it2=iis2.begin();
     for(i=1; i<r; i++)
```

```
     {
        same=same&&((*it1)==(*it2));
        it1++; it2++;
     }
     if(s1<s2) it2++; else it1++;
     for(i=r; i<(s-1); i++)
     {
        same=same&&((*it1)==(*it2));
        it1++; it2++;
     }
     if(s1<s2) it1++; else it2++;
     for(i=s; i<K; i++)
     {
        same=same&&((*it1)==(*it2));
        it1++; it2++;
     }
     return same;
}
void SetAb(list<int> hh)
{
     list<int> ii1,ii2,iis1,iis2,DD;
     list<int>::iterator itii1,itii2,its1,its2,ith;
     int i,i1,i2,s1,s2,j1,j2,jj1,jj2,K=hh.size();
     SetNus(hh);
     Nu=NuSum[K];
     SetDD(DD,0,hh);
     for(i1=1; i1<=Nu; i1++)
     {
        SetBlockIndices(i1,s1,j1);
        SetList(iis1,j1,s1,hh);
        ii1.erase(ii1.begin(),ii1.end());
        copy(iis1.begin(),iis1.end(),inserter(ii1,ii1.begin()));
        itii1=ii1.begin(); advance(itii1,s1-1);
        ii1.insert(itii1,0); itii1--;
        b[i1]=0;
        ith=hh.begin(); advance(ith,s1-1);
        for(i=1; i<=L[(*ith)]; i++)//set b
        {
```

```
   (*itii1)=i;
   jj1=Address(ii1,DD);
   b[i1]+=V(hh,jj1)*Ybar_dot(hh,jj1);
}
for(i2=1; i2<=i1; i2++)
{
   SetBlockIndices(i2,s2,j2);
   SetList(iis2,j2,s2,hh);
   ii2.erase(ii2.begin(),ii2.end());
   copy(iis2.begin(),iis2.end(),inserter(ii2,ii2.begin()));
   itii2=ii2.begin(); advance(itii2,s2-1);
   ii2.insert(itii2,0); itii2--;
   ith=hh.begin(); advance(ith,s2-1);
   if(s1==s2)//set diagonal block element
   {
      if(j1!=j2) A[i1][i2]=0;
      else
      {
          A[i1][i2]=0;
          for(i=1; i<=L[(*ith)]; i++)
          {
              (*itii2)=i;
              jj2=Address(ii2,DD);
              A[i1][i2]+=V(hh,jj2);
          }
      }
   }
   else //set off diagonal block element
   {
      if(!Compatible(iis1,iis2,s1,s2)) A[i1][i2]=0;
      else
      {
          its1=iis1.begin();
          its2=iis2.begin();
          advance(its2,s2-1);
          (s1<s2)? advance(its1,s2-2):advance(its1,s2-1);
          iis2.insert(its2,(*its1));
          jj2=Address(iis2,DD);
```

```
                  A[i1][i2]=V(hh,jj2);
              }
   }
        }//end for(i2
     }//end for(i1
}//end SetAb
void SolveLambda(void) //A is symmetric of dimension Nu x Nu
{// use Choleski decomposition A=GG' to solve A*lambda=b for lambda
 // First solves Gx=b for x and then solves x=G'lambda for lambda
 // x overwrites b, and G[i,j] overwrites A[i,j] for j<=i.
     int i,j,k;
     double sum;
     for(j=1; j<=Nu; j++)
       for(i=j; i<=Nu; i++)
       {
          sum=0;
          for(k=1; k<j; k++) sum+=A[i][k]*A[j][k];
          if(i==j) A[i][i]=sqrt(A[i][i]-sum);
          else A[i][j]=(A[i][j]-sum)/A[j][j];
       }//lower triangular G[i,j] overwrites A[i,j] for j<=i
       for(i=1; i<=Nu; i++)
       {
          sum=0;
          for(k=1; k<=(i-1); k++) sum+=b[k]*A[i][k];
          b[i]=(b[i]-sum)/A[i][i];
       }// b overwritten by x
       for(i=Nu; i>=1; i--)
       {
          sum=0;
          for(k=(i+1); k<=Nu; k++) sum+=A[k][i]*lambda[k];
          lambda[i]=(b[i]-sum)/A[i][i];
       }
}
bool InRange(list<int> is, int k, list<int> h)
{//returns true if is(k) is in range, otherwise false
     bool inLimit=true;
     int i, Lim, K=h.size();
     list<int>::iterator its, ith;
```

```
     ith=h.begin(); its=is.begin();
     for(i=1; i<K; i++)
     {
        if(i==k) ith++;
        Lim=((i<k)? L[(*ith)]-1 : L[(*ith)]);
        inLimit=inLimit&&((*its)<=Lim);
        its++; ith++;
     }
     return inLimit;
}
double LambdaSum(list<int> hh, int j)
{
     int jj,k,K=hh.size(),Lim;
     double LamSum=0;
     list<int> DDk,ii,iis;
     list<int>::iterator its,ith;
     SetList(ii,j,0,hh);
     SetAb(hh);
     SolveLambda();
     for(k=1; k<=K; k++)
     {
        iis.erase(iis.begin(),iis.end());
        copy(ii.begin(),ii.end(),inserter(iis,iis.begin()));
        its=iis.begin(); advance(its,k-1);
        iis.erase(its);
        SetDD(DDk,k,hh);
        if(InRange(iis,k,hh))
        {
           jj=NuSum[k-1]+Address(iis,DDk);
           LamSum+=lambda[jj];
        }
     }
     return LamSum;
}
double SS(list<int> hh)
{
     int j,MM=1;
     list<int>::iterator it;
```

```
     list<int>  ii;
     double ssh=0;
     InitializeList(ii,hh);
     for(it=hh.begin(); it!=hh.end(); it++) MM*=L[(*it)];
     for(j=1; j<=MM; j++)
       ssh+=V(hh,j)*sqr(Ybar_dot(hh,j)-LambdaSum(hh,j));
     return ssh;
}
int DF(list<int> hh)
{
     int df=1;
     list<int>::iterator it;
     for(it=hh.begin(); it!=hh.end(); it++) df*=(L[(*it)]-1);
     return df;
}
int DFe(void)
{
     if(N==M) return DF(Hp);
     return N-M;
}
double SSe(void)
{
     double sse=0;
     int i,j;
     if(N>M)
       for(i=1; i<=M; i++)
         for(j=1; j<=n[i]; j++) sse+=sqr(Y[i][j]-Ybar[i]);
     else sse=SS(Hp);
     return sse;
}
double SST(void)
{
     double Ysum=0,Ydotdot,sst=0;
     int i,j;
     for(i=1; i<=M; i++) for(j=1; j<=n[i]; j++) Ysum+=Y[i][j];
     Ydotdot=Ysum/N;
     for(i=1; i<=M; i++)
        for(j=1; j<=n[i]; j++) sst+=sqr(Y[i][j]-Ydotdot);
```

```
     return sst;
}
void PrintANOVA(void)
{
     bool start=true;
     list<int> H;
     cout<<"\n\n                        ";
     cout<<"ANALYSIS OF VARIANCE TABLE\n";
     if(N==M)
     {
        cout<<"One observation per cell. ";
        cout<<" The error sum of squares is\n";
        cout<<"calculated assuming the ";
        PrintList(Hp,' '); cout<<"interaction is zero.\n";
     }
     double ssH,sse,ssT,msH,mse,msT,FF,x,Pval;
     int i, k, dfH, dfe, dfT, last_i=(1<<p)-1;
     dfe=DFe(); sse=SSe(); mse=sse/dfe;
     dfT=N-1; ssT=SST(); msT=ssT/dfT;
     cout<<"\n";
     cout<<setfill('=')<<setw(58+2*p)<<"="<<"\n"<<setfill(' ');
     cout<<" Source "<<setw(2*p)<<" ";
     cout<<"          SS      D.F.       MS       F    P-value \n";
     cout<<setfill('=')<<setw(58+2*p)<<"="<<"\n"<<setfill(' ');
     Initialize(H);
     k=0; i=0;
     do //main effect and interaction entries
     {
        i++;
        if((i!=last_i)||(N>M))
        {
           start=(k<H.size());
           if(start)
           {
              k=H.size();
              if(k==1) cout<<"Main Effects______";
              else cout<<k<<"-way Interactions";
              cout<<setfill('_')<<setw(40+2*p)<<"_"<<"\n";
```

```
            cout<<setfill(' ');
         }
         cout<<((k==1) ? "Factor  ":"Factors ");
         PrintList(H,' ');
         ssH=SS(H); dfH=DF(H); msH=ssH/dfH;
         FF=msH/mse; x=sse/(ssH+sse);
         Pval=cdf::icbeta(x,dfe/2.0,dfH/2.0);
         cout<<setprecision(4)<<fixed<<setw(2*(p-k)+2)<<" ";
         cout<<setw(11)<<ssH<<"  ";
         cout<<setw(3)<<dfH<<"  "<<setw(10)<<msH<<"  ";
         cout<<setw(8)<<FF<<"  "<<setw(6)<<Pval<<"\n";
      }
   }while(Change(H));//next do error and total entries
   cout<<setfill('_')<<setw(58+2*p)<<"_"<<"\n"<<setfill(' ');
   cout<<"Error       "<<setw(2*p)<<" "<<setw(11)<<sse<<"  ";
   cout<<setw(3)<<dfe;
   cout<<"  "<<setw(10)<<mse<<"\n";
   cout<<setfill('=')<<setw(58+2*p)<<"="<<"\n"<<setfill(' ');
   cout<<"Total       "<<setw(2*p)<<" "<<setw(11)<<ssT<<"  ";
   cout<<setw(3)<<dfT;
   cout<<"  "<<setw(10)<<msT<<"\n";
}
void CleanUp(void)
{
   int i;
   for(i=1; i<=M; i++)
   { delete[] Y[i]; delete[] A[i];}
   delete[] A; delete[] b; delete[] lambda;
   delete[] Y; delete[] Ybar; delete[] n;
   delete[] L; delete[] nu; delete[] NuSum;
}
int main(int argc, char *argv[])
{
   GetData(argv[1]);
   SetWeights();
   SetStorage();
   SetYbar_N();
   PrintData();
```

```
    PrintANOVA();
    CleanUp();
    return 0;
}
```

Appendix J

C++ program for the Wilcoxon signed rank distribution

```
//Wilcox.h Subroutines for Wilcoxon one sample signed rank test
#include <cmath>
#include <vector>
#include <list>
#include <iterator>
#include <algorithm>

using namespace std;

namespace sRank
{
  class node
  {
    public:
    int w;
    double pr;
    node(int c=0, double d=0):w(c),pr(d) {}
    bool operator ==(const node &y) const
    { return w==y.w;}
    bool operator < (const node &y) const
    { return w<y.w;}
  };
```

```
int n,K,*a;
list<node> *sRankList;

double bin(int x, int m) // binomial(x,m,1/2)=mCx/2^m density
{
  double r, dx=(double)x, dm=(double)m, sum=-dm*log(2.0);
  for(r=dx; r>0; r--) sum+=log(dm--/r);
  return exp(sum);
}

void Set_nKa(vector<int> t)
{
  int k;
  K=t.size()-1;
  n=0; for(k=0; k<=K; k++) n+=t[k];
  a=new int[K+1];
  a[0]=t[0]+1; for(k=1; k<=K; k++) a[k]=a[k-1]+t[k-1]+t[k];
}


void SetNodes(int W, vector<int> t)
{
  node nd;
  int nk,w,uk,k,wk,Mk,Bk;
  list<node>::iterator it,itf;
  Set_nKa(t);
  Bk=n*(n+1)-t[0]*(t[0]+1);
  Mk=Bk/2;
  nd.w=W; nd.pr=0;
  sRankList=new list<node>[K+1];
  sRankList[K].push_back(nd);
  nk=n;
  for(k=K-1; k>=0; k--)
  {
    nk-=t[k+1];
    Bk=nk*(nk+1)-t[0]*(t[0]+1); Mk=Bk/2;
    for(it=sRankList[k+1].begin(); it!=sRankList[k+1].end(); it++)
    {
```

```
      w=it->w;
      for(uk=0; uk<=t[k+1]; uk++)
      {
        wk=w-a[k+1]*uk;
if(wk>Mk) wk=Bk-wk-1;
nd.w=wk;
itf=find(sRankList[k].begin(),sRankList[k].end(),nd);
if((wk>=0)&&(itf==sRankList[k].end()))  sRankList[k].push_back(nd);
      }
    }
  }
}//end SetNodes

double  Prob(int W, vector<int> t)
{
  bool complement;
  int k,w,uk,wk,Mk,Bk,nk;
  double sum, Prob;
  list<node>::iterator it,it1;
  SetNodes(W,t);
  for(it=sRankList[0].begin(); it!=sRankList[0].end(); it++) it->pr=1.0;
  nk=0;
  for(k=0; k<K; k++)
  {
    nk+=t[k]; Bk=nk*(nk+1)-t[0]*(t[0]+1); Mk=Bk/2;
    for(it=sRankList[k+1].begin(); it!=sRankList[k+1].end(); it++)
    {
      w=it->w; sum=0;
      for(uk=0; uk<=t[k+1]; uk++)
      {
        wk=w-uk*a[k+1];
if(wk>Mk)
{
  wk=Bk-wk-1;
  complement=true;
}
else complement=false;
if(wk>=0)
```

```
  {
    for(it1=sRankList[k].begin(); it1!=sRankList[k].end(); it1++)
     if((it1->w)==wk) break;
    if(!complement) sum+=(it1->pr)*bin(uk,t[k+1]);
    else sum+=(1.0-it1->pr)*bin(uk,t[k+1]);
  }
  else if(complement) sum+=bin(uk,t[k+1]);
        }
        it->pr=sum;
      }
    }
    it=sRankList[K].begin();
    Prob=it->pr;
    delete[] sRankList;
    return Prob;
  }//end Prob
}//end namespace sRank
```

Appendix K

C++ program to calculate the P-value using the Wilcoxon signed rank test

```
// sRank.cpp Program to compute W+ the Wilcoxon signed rank statistic.
// It calculates the value w for W+ from a given set of data. It has
// provision for zeros and ties (t[0] is the number of zeros
// and t[1],t[2],...,t[K] are the number tied for the magnitude
// ranks in increasing order 1,2,...,K. u[k] are the number of
// postiive observations with magnitude rank k). The statistic
//            W+ =u[1]a[1]+u[2]a[2]+...u[K]a[K]
// where a[k]=t[0]+...+a[k-1]+(a[k]+1)/2 are average ranks.
// If the sample size n<=200 it calculates the exact P-values
// P(W+<=w |K,(t[0],t[1],...,t[K}) and P(W+>=w|K,t).
// Approximate P-values are calculated using the normal approximation.
// Copyright (C) 2004 Jetrome H. Klotz, University of Wisconsin.
#include <iostream>
#include <fstream>
#include <stdlib.h>
#include <cmath>
#include <vector>
#include <list>
#include <iterator>
#include <algorithm>
#include <iomanip>
```

```
#include "normal.h"
#include "Wilcox.h"

using namespace std;

int i,j,W,K,n;
vector<int> u,t,a;


class pairtype
{
  public:
   double x; //for Xi i=1,2,...,n
   double z; //for|Xi|
   pairtype(double r=0, double s=0): x(r),z(s) {}
   bool operator == (const pairtype &y) const
   { return z==y.z;} //for sorting on |Xi|
   bool operator < (const pairtype &y) const
   { return z<y.z;}
};

vector<pairtype> XZ;

void GetData(char *filename)
{
  double V;
  pairtype R;
  ifstream infile;
  infile.open(filename);
  if(!infile)
  {
    cout<<"Cannot open "<<filename<<" for input.\n";
    exit(1);
  }
  do
  {
    XZ.push_back(R);
    infile>>V;
```

```
    R=pairtype(V,fabs(V));
  }
  while(!infile.eof());
  n=XZ.size()-1;
  sort(XZ.begin(),XZ.end());
}

void Set_ut()
{
  i=1;
  for(j=0; j<=n; j++)
  {
    t.push_back(0);
    u.push_back(0);
    if(j==0)
     while((i<n)&&(XZ[i].z==0))
     {
       t[0]++; i++;
     }
    else
     {
       t[j]++;
       if(XZ[i].x>0) u[j]++;
       while((i<n)&&(XZ[i].z==XZ[i+1].z))
       {
         t[j]++;
         if(XZ[i+1].x>0) u[j]++;
         i++;
       }
       i++;
     }
     if(i>n) break;
  }
  K=t.size()-1;
}

void Set_a()
{
```

```
  a.push_back(t[0]+1);
  for(i=1; i<=K; i++) a.push_back(a[i-1]+t[i-1]+t[i]);
}

void SetW()
{
  W=0;
  for(i=1; i<=K; i++) W+=a[i]*u[i];
}


void ApproxPval()
{
  int k,sum0=0;
  double z, EW, VarW, sum1=0;
  double alpha0,alpha1,alpha2;
  EW=(double)(n*(n+1)-t[0]*(t[0]+1))/2;
  for(k=1; k<=K; k++) sum0+=t[k]*(t[k]-1)*(t[k]+1);
  sum1=(double)(n*(n+1)*(2*n+1)-t[0]*(t[0]+1)*(2*t[0]+1));
  VarW=(sum1/6.0) -((double)sum0)/12.0;
  z=((double)W-EW)/sqrt(VarW);
  alpha0=Phi(z);
  alpha1=1-Phi(z);
  alpha2=2*min(alpha0,alpha1);
  cout<<"Normal approximation with zeros and ties correction \n\n";
  cout<<"Approximate lower tail P-value "<<setprecision(4)<<alpha0<<".\n\n";
  cout<<"Approximate upper tail P-value "<<alpha1<<".\n\n";
  cout<<"Approximate two tailed P-value "<<alpha2<<".\n\n";
  cout<<"E(W+)= "<<setw(7)<<EW/2.0<<" , Var(W+)= "<<setw(7)<<VarW/4.0<<", ";
  cout<<"z= "<<setprecision(5)<<z<<" .\n\n";
}

void PrintHeading(char *filename)
{
  double Wplus=(double)W/2.0;
  cout<<"\n\nWilcoxon signed rank test for data in "<<filename<<" .\n\n";
  cout<<"Average magnitude ranks are used with zeros and ties.\n";
  cout<<"Zeros are used to form average magnitude ranks with\n";
```

```
  cout<<"W+ the sum of these ranks for positive observations.\n\n";
  cout<<"W+="<<Wplus<<" for sample size n= "<<n<<".\n\n";
}

void PrintAnswers()
{
  double PWKt,PBk_WKt;
  int W2=n*(n+1)-t[0]*(t[0]+1)-W;
  PWKt=sRank::Prob(W,t);
  PBk_WKt=sRank::Prob(W2,t);
  double Wplus=(double)W/2.0;
  double alpha2=2.0*min(PWKt,PBk_WKt);
  cout<<"Lower tail P-value  P(W+<="<<Wplus<<" |"<<K<<",t)= ";
  cout<<setprecision(12)<<PWKt<<"\n\n";
  cout<<"Upper tail P-value P(W+>="<<Wplus<<" |"<<K<<",t)= ";
  cout<<setprecision(12)<<PBk_WKt<<"\n\n";
  cout<<"Two sided P-value= "<<alpha2<<" .\n\n";
}

int main(int argc, char *argv[])
{
  GetData(argv[1]);
  Set_ut();
  Set_a();
  SetW();
  PrintHeading(argv[1]);
  if(n<=200)
   PrintAnswers();
  ApproxPval();
  return 1;
}
```

Appendix L

C++ subroutine to calculate the Mann Whitney Wilcoxon distribution with ties

```
// MannW2.h Subroutine for Mann Whitney Wilcoxon two sample rank test distribution
#include <vector>
#include <list>
#include <iterator>
#include <algorithm>
#include "cdf.h"

using namespace std;

namespace MannW
{

class type3
{
    public:
     int m;  // X sample size
     int u2; // statistic value
     double pr; // probability value
     type3(int c=0, int d=0, int e=0):m(c),u2(d),pr(e) {}
     bool operator == (const type3 &y) const
     { return (m==y.m)&&(u2==y.u2);} //for finding (m,u2) values
```

```
     bool operator < (const type3 &y) const
     { return ((m<y.m)||((m==y.m)&&(u2<y.u2)));}
};

list<type3> *A;
int  *a, K, N;

void Set_aKN(vector<int> t)
  {
    int i;
    K=t.size()-1;
    a=new int[K+1];
    N=t[1]; a[1]=t[1];
    for(i=2; i<=K; i++)
    {
      N+=t[i]; a[i]=a[i-1]+t[i-1]+t[i];
    }
  }

void PrintList(list<type3> L)
{
  int count=0;
  list<type3>::iterator it3;
  cout<<"(m,u2,pr)) values:\n";
  for(it3=L.begin(); it3!=L.end(); it3++)
  {
    count++;
    cout<<"("<<it3->m<<", "<<it3->u2<<", "<<it3->pr<<"), ";
    if(count%8==0) cout<<"\n";
  }
  cout<<"\n";
}

int Umin(int k, int m, vector<int> t)
{
  int ui, U2=-m*m, mk=m;
  for(int i=1; i<=k; i++)
  {
```

```
    ui=min(mk,t[i]);
    mk-=ui;
    U2+=ui*a[i];
  }
  return U2;
}

int Umax(int k, int m, vector<int> t)
{
  int ui, U2=-m*m, mk=m;
  for(int i=k; i>0; i--)
  {
    ui=min(mk,t[i]);
    mk-=ui;
    U2+=ui*a[i];
  }
  return U2;
}

void SetList(int U2, int m, vector<int> t)
{
    int k,mk,mk1,rk,Lower_k,Upper_k,sum_tk;
    int u2k, u2k1;
    list<type3>::iterator it3,it30;
    Set_aKN(t);
    A=new list<type3>[K+1];
    type3 T3;
    T3.m=m; T3.u2=U2; T3.pr=0;
    A[K].push_back(T3);
    sum_tk=N;
    for(k=K-1; k>1; k--)
    {
      sum_tk-=t[k+1];
      for(it3=A[k+1].begin(); it3!=A[k+1].end(); it3++)
      {
        mk=it3->m; u2k=it3->u2;
Lower_k=max(0,mk-sum_tk); Upper_k=min(mk,t[k+1]);
for(rk=Lower_k; rk<=Upper_k; rk++)
```

```
{
  u2k1=u2k-rk*(a[k+1]-2*mk+rk);
  mk1=mk-rk; T3.m=mk1; T3.u2=u2k1;
  if((u2k1>=Umin(k,mk1,t))&&(u2k1<=Umax(k,mk1,t)))
  {
    it30=find(A[k].begin(),A[k].end(),T3);
    if(it30==A[k].end()) A[k].push_back(T3);
          }
}
      }
    }
}

void CleanUp(void)
{
   int k;
   for(k=0; k<=K; k++) A[k].erase(A[k].begin(),A[k].end());
   delete[]A;
}

double Prob(int U2, int m, vector<int> t)
{
  int x, k, u20, u2k, rk, m0, mk;
  int sum_tk1, N2, Nk, Lower_k, Upper_k;
  double ProbSum;
  type3 T3;
  list<type3>::iterator it3,it31;
  SetList(U2,m,t);
  if(K<2) { cout<<"K<2, exit.\n"; exit(0);}
  if(K==2)
  {
    x=(U2-m*(t[1]-m))/N;
    return CDF::HyperG(x,N,t[2],m);
  }
  N2=t[1]+t[2];
  for(it3=A[2].begin(); it3!=A[2].end(); it3++)
  {
    m0=it3->m; u20=it3->u2;
```

```
    x=(u20-m0*(t[1]-m0))/N2;
    it3->pr=CDF::HyperG(x,N2,t[2],m0);
  }
  sum_tk1=t[1];
  for(k=3; k<=K; k++)
  {
    sum_tk1+=t[k-1]; Nk=sum_tk1+t[k];
    for(it3=A[k].begin(); it3!=A[k].end(); it3++)
    {
      m0=it3->m; u20=it3->u2;
      ProbSum=0;
      Lower_k=max(0,m0-sum_tk1); Upper_k=min(m0,t[k]);
      for(rk=Lower_k; rk<=Upper_k; rk++)
      {
        u2k=u20-rk*(a[k]-2*m0+rk); mk=m0-rk;
T3.m=mk; T3.u2=u2k;
if( (Umin(k-1,mk,t)<=u2k)&&(u2k<=Umax(k-1,mk,t)) )
{
   it31=find(A[k-1].begin(),A[k-1].end(),T3);
   ProbSum+=(it31->pr)*CDF::p(rk,Nk,t[k],m0);
}
else if(Umax(k-1,mk,t)<u2k) ProbSum+=CDF::p(rk,Nk,t[k],m0);
      }
      it3->pr=ProbSum;
    }
  }
  it3=A[K].begin();
  ProbSum=it3->pr;
  CleanUp();
  return ProbSum;
}

}//end namespace MannW
```

Appendix M

C++ program to calculate approximate and exact ($N \leq 100$) P-values for the Wilcoxon two sample rank test.

```
//RankSum.cpp Program to compute the P-value for the two
//sample Wilcoxon Mann Whitney rank sum test.
#include <iostream>
#include <fstream>
#include <iomanip>
#include <cmath>
#include <vector>
#include <iterator>
#include <algorithm>
#include "MannW.h"  //Appendix M
#include "normal.h" //Appendix G

using namespace std;

int m,n,N,K,U2;
double UYX;
vector<double> X,Y;
vector<int> u,t,a;
```

```
class pairtype
{
  public:
   int z;
   double Z;
   pairtype(int c=0, double d=0): z(c), Z(d) {}
   bool operator == (const pairtype &y) const
   { return Z==y.Z;}
   bool operator < (const pairtype &y) const
   { return Z<y.Z;}
} T2;

vector<pairtype> zZ;

int ReadFile(char *filename, vector<double> &W)
{
  double V=0;
  ifstream infile;
  infile.open(filename);
  if(!infile)
  { cout<<"Cannot open "<<filename<<" for input.\n"; exit(0);}
  do
  {
    W.push_back(V);
    infile>>V;
  } while(!infile.eof());
  infile.close();
  return W.size()-1;
}

void GetData_mn(char *filename1, char *filename2)
{
  m=ReadFile(filename1,X);
  n=ReadFile(filename2,Y);
}

void SetNzZ()
{
```

```
  int k;
  N=m+n;
  for(k=1; k<=N; k++)
  {
    if(k<=m) { T2.z=1; T2.Z=X[k];}
    else { T2.z=0; T2.Z=Y[k-m];}
    zZ.push_back(T2);
  }
}

void SetKtua()
{
  int i,k=1;
  sort(zZ.begin(), zZ.end());
  u.push_back(0); t.push_back(0);
  u.push_back(zZ[0].z); t.push_back(1);
  for(i=1; i<N; i++)
  {
    if(zZ[i-1].Z==zZ[i].Z)
    { t[k]++; u[k]+=zZ[i].z;}
    else
    {
      k++; t.push_back(1);
      u.push_back(zZ[i].z);
    }
  }
  K=t.size()-1;
  a.push_back(0);
  for(i=1; i<=K; i++) a.push_back(a[i-1]+t[i-1]+t[i]);
}

void SetU2()
{
  int k;
  U2=-m*m;
  for(k=1; k<=K; k++) U2+=u[k]*a[k];
  UYX=((double)U2)/2.0;
}
```

```
void PrintHeading(char *filename1, char *filename2)
{
  cout<<"P-values for the Wilcoxon Mann Whitney two sample ";
  cout<<"rank sum test for the \n";
  cout<<"X sample data in file ‘"<<filename1<<"’ and the ";
  cout<<"Y sample data in file ‘"<<filename2<<"’.\n\n";
}

void PrintExact()
{
  int i, C1=min(U2,2*m*n-U2),C2=max(U2,2*m*n-U2), count=0;
  double dC1=((double)C1)/2.0, dC2=((double)C2)/2.0;
  double alphaL=MannW::Prob(U2,m,t);
  double alphaU=1.0-MannW::Prob(U2-1,m,t);
  double alpha2=MannW::Prob(C1,m,t)+1.0-MannW::Prob(C2-1,m,t);
  cout<<"Using the exact distribution: \n";
  cout<<"UYX = "<<UYX<<", m= "<<m<<", n= "<<n<<"\n";
  cout<<"Lower tail P-value is P(UYX<="<<UYX<<"|m, t)= ";
  cout<<alphaL<<"\n";
  cout<<"Upper tail P-value is P(UYX>="<<UYX<<"|m, t)= ";
  cout<<alphaU<<"\n";
  cout<<"For the two sided test which rejects for ";
  cout<<"|UYX-E(UYX)|>=C \n";
  cout<<"the P-value is P(UYX<="<<dC1<<"|m,t)+P(UYX>=";
  cout<<dC2<<"|m,t)= "<<alpha2<<" .\n";
}

void PrintApprox()
{
  int i, count=0, c=0;
  double EUYX, VarUYX,sigmaUYX, Z;
  double dm=(double)m, dn=(double)n, dN=(double)N, dc;
  double alphaL,alphaU, alpha2;
  EUYX=dm*dn/2.0;
  for(i=1; i<=K; i++) c+=(t[i]-1)*t[i]*(t[i]+1);
  dc=(double)c; // tie correction factor
  VarUYX=dm*dn*(dN+1.0)*(1.0-dc/((dN-1.0)*dN*(dN+1)))/12.0;
```

```
  sigmaUYX=sqrt(VarUYX);
  Z=(UYX-EUYX)/sigmaUYX;
  alphaL=Phi(Z); alphaU=1.0-alphaL;
  alpha2=2.0*min(alphaL,alphaU);
  cout<<"\nUsing the normal approximation with\n";
  cout<<"UYX = "<<UYX<<", m= "<<m<<", n= "<<n<<"\n";
  cout<<"E(UYX)="<<EUYX<<", Var(UYX)="<<VarUYX<<;
  cout<<", sigma(UYX)="<<sigmaUYX<<"\n";
  cout<<"Z=(UYX-E(UYX))/sigma(UYX)="<<Z<<"\n";
  cout<<"Approximate lower tail P-value is ";
  cout<<setw(7)<<alphaL<<"\n";
  cout<<"Approximate upper tail P-value is ";
  cout<<setw(7)<<alphaU<<"\n";
  cout<<"Approximate P-value for the two sided test is ",
  cout<<setw(7)<<alpha2<<"\n";
  cout<<"for ties\nt=(";
  for(i=1; i<K; i++)
  {
    count++; cout<<t[i]<<", ";
    if(count%30==0) cout<<"\n";
  }
  cout<<t[K]<<").\n";
  cout<<"K= "<<K<<", sum(t[i]^3-t[i])= "<<c<<" .\n";
}

int main(int argc, char *argv[])
{
  PrintHeading(argv[1],argv[2]);
  GetData_mn(argv[1],argv[2]);
  SetNzZ();
  SetKtua();
  SetU2();
  if(N<=100) PrintExact();
  PrintApprox();
  return 1;
}
```

Appendix N

C++ program to calculate the P-value for the Mood and Brown K sample Median Test.

```
//Mood.cpp Program for the Mood and Brown test.
//Copyright (C) 2002 H.S. Jorn and J.H. Klotz
#include<iostream>
#include<fstream>
#include<string>
#include<vector>
#include<algorithm>
#include<iomanip>
#include<cmath>
#include<ctime>
#define sqr(x) ((x)*(x))

using namespace std;

//global variables
vector<int> n_vec; //for sample sizes
vector<int> m_vec; //for counts above median
vector<double> z;  //for data values
int K,a;           //number of samples, total observations, sum m[i]
double da;         //double version of a
int *n,*m,*N;      //n[i] sample sizes, m[i] counts above median,
```

```
double *dN,*dm,*dn;//double versions of N[i],m[i],n[i]
double **X,median; //X[i][j] are data values, median of pooled samples
bool data_entered; //true if values entered, false if counts entered
double V0,Chi2;    //statistics for data
double *lnInt;    //(ln(1), ln(2),...,ln(N[K])
long counts=0;     //number of nodes modified
bool writeFile;    //true if output file desired, false otherwise
bool valuedata;    //true if values entered
string fname;      //name of output file
ofstream ofile;    //output file
time_t  startTime, endTime;//for timing the calculation in seconds
clock_t startTick, endTick;//for timing clock ticks of the computer

class node
{
  public:
   double vk, Qk;
   int ak,mk;
   node(double v0=0, double Q0=0, int a0=0, int m0=0):
    vk(v0), Qk(Q0), ak(a0), mk(m0){}//constructor
    node& node::operator=(const node &r)
    {//to set one node = another
      if(&r!=this)
      {
        vk=r.vk; Qk=r.Qk; ak=r.ak; mk=r.mk;
      }
      return *this;
    }
} *A;//for Array[1,...,K] of nodes

void getKeyData()
{
  int i,j, nival;
  double x;
  cout<<"Enter the number of rows K :";
  cin>>K;
  cout<<"Enter the number of data values per row :";
  n_vec.push_back(0);
```

```
  for(i=1; i<=K; i++)
  {
    cin>>nival;
    n_vec.push_back(nival);
  }
  cout<<"Enter data matrix (X[i,j]) by rows #i=1,2";
  if(K>3) cout<<",...,";
  if(K==3) cout<<",";
  if(K>2) cout<<K<<"\n";
  for(i=1; i<=K; i++)
  {
    cout<<"row #"<<i<<": ";
    for(j=1; j<=n_vec[i]; j++)
    {
      cin>>x;
      z.push_back(x);
    }
  }
}

void getFileData()
{
  int i, j, nival;
  string filename;
  double x;
  cout<<"Enter input data file name: ";
  cin>>filename;
  cout<<"File name "<<filename<<" obtained\n";
  ifstream infile(filename.c_str());
  if(!infile)
  {
    cout<<"Cannot open input file "<<fname<<"\n";
    exit(0);
  }
  infile>>K;
  n_vec.push_back(0);
  for(int i=1; i<=K; i++)
  {
```

```
    infile>>nival;
    n_vec.push_back(nival);
  }
  for(i=1; i<=K; i++)
    for(j=1; j<=n_vec[i]; j++)
    {
      infile>>x;
      z.push_back(x);
    }
  infile.close();
}

void getData()
{
  char ch;
  cout<<"Do you wish to enter data from the keyboard or from a file?\n";
  do
  {
    cout<<"Type K for keyboard or F for file : ";
    cin>>ch;
    if(ch=='K'||ch=='k') getKeyData();
    else if(ch=='F'||ch=='f') getFileData();
  } while(!(ch=='K'||ch=='k'||ch=='F'||ch=='f'));
}

void getKeyCounts()//for entering counts by keyboard
{
  int i,ni,mi;
  cout<<"Enter the number of samples K : ";
  cin>>K;
  cout<<"Enter counts above median m[i] for i=1,2";
  if(K>3) cout<<",...,";
  if(K==3) cout<<",";
  if(K>2) cout<<K;
  cout<<"\n:  ";
  m_vec.push_back(0);
  for( i=1; i<=K; i++)
  {
```

```
    cin>>mi;
    m_vec.push_back(mi);
  }
  cout<<"Enter sample sizes n[i], i=1,2";
  if(K>3) cout<<",...,";
  if(K==3) cout<<",";
  if(K>2) cout<<K;
  cout<<"\n:  ";
  n_vec.push_back(0);
  for( i=1; i<=K; i++)
  {
    cin>>ni;
    n_vec.push_back(ni);
  }
}

void getFileCounts()
{
  int ci, i, j;//counts
  string filename;
  cout<<"For a count file (first row number of samples, second row counts above media
  cout<<"third row sample sizes),\n";
  cout<<"enter input count file name : ";
  cin>>filename;
  ifstream infile(filename.c_str());
  if(!infile)
  {
    cout<<"Cannot open input file "<<filename<<"\n";
    exit(0);
  }
  infile>>K;
  m_vec.push_back(0);
  n_vec.push_back(0);
  for(i=1; i<=2; i++)
    for(j=1; j<=K; j++)
    {
      infile>>ci;
      if(i==1) m_vec.push_back(ci);
```

```
      else n_vec.push_back(ci);
    }
  cout<<"Counts entered.\n";
  infile.close();
}

void getCounts()
{
  char ch;
  cout<<"Do you wish to enter counts from the keyboard or from a file?\n";
  do
  {
    cout<<"Type K for keyboard or F for file : ";
    cin>>ch;
    if(ch=='K'||ch=='k') getKeyCounts();
    else if(ch=='F'||ch=='f') getFileCounts();
  } while(!(ch=='K'||ch=='k'||ch=='F'||ch=='f'));
}

void printData()
{
  cout<<"\nData matrix:\n";
  for(int i=1; i<=K; i++)
  {
    for(int j=1; j<=n[i]; j++) cout<<X[i][j]<<" ";
    cout<<"\n";
  }
  cout<<"\n\n";
}

void printCounts(bool valdata)
{
  int i;
  cout<<"Sample counts m[i] of values above pooled median,\n";
  cout<<"and sample sizes n[i], for i=1,2";
  if(K>3) cout<<",...,";
  if(K==3) cout<<",";
  if(K>2) cout<<K<<".\n\n";
```

```
  if(K==2) cout<<".\n\n";
  cout<<" #i |";
  for(i=1; i<=K; i++) { cout<<setw(4)<<i<<" "; }
  cout<<" | Total\n";
  for(i=0; i<=K+2; i++) cout<<"_____";
  cout<<"\n";
  cout<<"m[i]|";
  for(i=1; i<=K; i++) { cout<<setw(4)<<m[i]<<" ";}
  cout<<" | "<<setw(4)<<a<<"\n";
  for(i=0; i<=K+2; i++) cout<<"_____";
  cout<<"\n";
  cout<<"n[i]|";
  for(i=1; i<=K; i++) { cout<<setw(4)<<n[i]<<" ";}
  cout<<" | "<<setw(4)<<N[K]<<"\n";
  for(i=0; i<=K+2; i++) cout<<"_____";
  cout<<"\n\n";
  if(valdata) cout<<"Median of pooled sample is "<<median<<" .\n\n";
}

void getInput()
{
  char ch;
  cout<<"Do you wish to enter data vaues or counts?\n";
  do
  {
    cout<<"Type V for data values or C for counts : ";
    cin>>ch;
    if(ch=='V'||ch=='v')
    {
      data_entered=true;
      getData();
      valuedata=true;
    }
    else if(ch=='C'||ch=='c')
    {
      data_entered=false;
      getCounts();
      valuedata=false;
```

```
    }
  } while(!(ch=='V'||ch=='v'||ch=='C'||ch=='c'));
}

void writeData(ostream &file)
{
  int i,j;
  file<<"The data values are :\n";
  for(i=1; i<=K; i++)
  {
    for(j=1; j<=n[i]; j++) file<<X[i][j]<<" ";
    file<<"\n";
  }
  file<<"The combined samples median is    : "<<median<<"\n";
}

void writeCounts(ostream &file)
{
  int i;
  file<<"Sample sizes for "<<K<<" samples        : n=( ";
  for(i=1; i<K; i++) file<<setw(3)<<n[i]<<", ";
  file<<setw(3)<<n[K]<<").\n";
  file<<"Corresponding Counts above median : m=( ";
  for(i=1; i<K; i++) file<<setw(3)<<m[i]<<", ";
  file<<setw(3)<<m[K]<<").\n";
}

void printInput()
{
  char ch;
  bool ok;
  if(data_entered) printData();
  printCounts(valuedata);
  cout<<"Do you wish to write answers to a file?\n";
  do
  {
    cout<<"Type y)es or n)o :";
    cin>>ch;
```

```
    ok=(ch=='y')||(ch=='Y')||(ch=='n')||(ch=='N');
  } while (!ok);
  if (ch=='y'||ch=='Y') writeFile=true;
  else writeFile=false;
  if(writeFile)
  {
    cout<<"Enter output data file name: ";
    cin>>fname;
    ofile.open(fname.c_str());// ,ios::app); to append
    if(!ofile)
    {
      cout<<"Can't open "<<fname<<" for writing.\n";
      exit(0);
    }
    if(data_entered) writeData(ofile);
    writeCounts(ofile);
    ofile.close();
  }
}

void print_K_n()
{
  int j;
  vector<int>::iterator itn,ite=n_vec.end();
  cout<<"K="<<K<<" rows. Row size vector n=(";
  if(K>0)
  {
    for(j=1; j<K; j++)
      cout<<n_vec[j-1]<<",}";
    cout<<n_vec[K-1];
  }
  else cout<<0;
  cout<<").\n\n";
}

void Allocate()
{
  n=new int[K+1];
```

```
  dn=new double[K+1];
  m=new int[K+1];
  dm=new double[K+1];
  N=new int[K+1];
  dN=new double[K+1];
  A=new node[K+1];
}

void setLnInt()
{
  lnInt=new double[N[K]+1];
  for(int i=1; i<=N[K]; i++) lnInt[i]=log((double)i);
}

void initialize()
{
  int i,j;
  vector<int>::iterator itn=n_vec.begin();
  vector<int>::iterator itm=m_vec.begin();
  vector<double>::iterator itz=z.begin();
  N[0]=0;
  itn++;
  for(i=1; i<=K; i++)
  {
    n[i]=*itn;
    dn[i]=(double)n[i];
    itn++;
    N[i]=N[i-1]+n[i];
    dN[i]=(double)N[i];
  }
  if(!data_entered)
  {
    a=0; itm++;
    for(i=1; i<=K; i++)
    {
      m[i]=*itm;
      dm[i]=(double)m[i];
      itm++;
```

```
      a+=m[i];
    }
  }
  else
  {
    X=new (double*)[K+1];
    for(i=1; i<=K; i++) X[i]=new double[n[i]+1];
    for(i=1; i<=K; i++)
      for(j=1; j<=n[i]; j++)
      {
        X[i][j]=*itz; itz++;
      }
    sort(z.begin(),z.end());
    int t=(N[K]/2)-1; //t is integer floor(N/2)-1 since z[0] is sorted X[1][1]
    if(N[K]%2) median=z[t+1];
    else median=(z[t]+z[t+1])/2.0; //overall median calculated
    a=0;
    for(i=1; i<=K; i++)
    {
      m[i]=0;
      for(j=1; j<=n[i]; j++)
      if(X[i][j]>median) m[i]++;
      dm[i]=(double)m[i];
      a+=m[i];
    }
  }
  da=(double)a;
  setLnInt();
}

void DeAllocate()
{
  delete[]n;
  delete[]dn;
  delete[]m;
  delete[]dm;
  delete[]N;
  delete[]dN;
```

```
  if(data_entered)
  {
    for(int i=1; i<=K; i++) delete[] X[i];
    delete[] X;
  }
  delete[] A;
  delete[] lnInt;
}

template <class T>
double Vstat(int k, T *u, int *n)
{ //returns v=u[1]^2/n[1]+...+u[k]^2/n[k]
  double v=0,du, dn;
  for(int i=1; i<=k; i++)
  {
    du=(double)u[i];
    dn=(double)n[i];
    v+=du*du/dn;
  }
  return(v);
}

double Chi2stat()
{
  double sum=0;
  for(int i=1; i<=K; i++) sum+=(sqr(dm[i]-da*dn[i]/dN[K]))/dn[i];
  sum*=dN[K]*(dN[K]-1)/(da*(dN[K]-da));
  return sum;
}

void setStats()
{
  V0=Vstat(K,m,n);
  Chi2=Chi2stat();
}


double Vmin(int k, int ak)
```

```
{
  return sqr(ak)/dN[k];
}


double lnP(int r, int k) // calculates ln(r_P_k) where r_P_k
{  // is the number of permutations of r things taken k at a time
  double sum=0;
  for(int i=k; i>0; i--) sum+=lnInt[r--];
  return sum;
}

double hyperG(int x, int n, int D, int N)//hypergeometric
{ // h(x;(n,D,N))=(n_C_x)*((N-n)_C_(D-x))/N_C_D probability
  double sum=lnP(n,x)+lnP(D,x)+lnP(N-D,n-x)-(lnP(x,x)+lnP(N,n));
  return exp(sum);
}

void printNodes()
{
  cout<<"Nodes:";
  for(int i=1; i<=K; i++)
    cout<<"("<<A[i].vk<<","<<A[i].Qk<<","<<A[i].ak<<","<<A[i].mk<<") ";
  cout<<"\n";
}

void setStartA()
{
  double vk=V0;
  int ak=a,mk;
  for(int i=K; i>0; i--)
  {
    mk=max(0,ak-N[i-1]);
    A[i].vk=vk;
    A[i].Qk=0;
    A[i].ak=ak;
    A[i].mk=mk;
    vk-=sqr(mk)/dn[i];
```

```
    ak-=mk;
  }
}

void resetA(int k)
{//resets A[1,2,...,k] using A[k+1]
  for(int i=k; i>0; i--)
  {
    A[i].vk=A[i+1].vk-sqr(A[i+1].mk)/dn[i+1];
    A[i].Qk=0;
    A[i].ak=A[i+1].ak-A[i+1].mk;
    A[i].mk=max(0,A[i].ak-N[i-1]);
  }
}

void setProb()
{
  int k=1;
  double epsilon=1.0e-8;
  do
  {
    if(k==1)
    {
      if(A[1].vk-epsilon<(sqr(A[1].ak)/dn[1])) A[1].Qk=1;
      else A[1].Qk=0;
      k++;
      counts++;
    }
    else
    {
      if(A[k].vk-epsilon<Vmin(k,A[k].ak)) A[k++].Qk=1;
      else
      {
        if(A[k-1].Qk>0)
        A[k].Qk+=A[k-1].Qk*hyperG(A[k].mk, A[k].ak, n[k], N[k]);
        if((A[k].mk)==(min(n[k],A[k].ak))) k++;
        else
        {
```

```
          A[k].mk++;
          resetA(k-1);
          k=1;
        }
      }
    }
  } while(k<=K);
}

void printAnswers()
{
  cout<<"\nThe Mood & Brown chi square statistic Chi^2= ";
  cout<<setprecision(5)<<Chi2<<"\n";
  cout<<"Equivalently, V=M[1]^2/n[1]+...+M[K]^2/n[K]= ";
  cout<<setprecision(5)<<V0<<" \n\n";
  cout<<setprecision(5)<<"The P-value P[V>="<<V0<<"]= ";
  cout<<setprecision(12)<<A[K].Qk<<"\n";
  cout<<"for K="<<K<<", n=(";
  for(int j=1; j<K; j++) cout<<n[j]<<", ";
  cout<<n[K]<<"), and  a="<<a<<".\n\n";
  cout<<"count="<<counts<<"\n\n";
}

void writeAnswer()
{
  int i;
  ofile.open(fname.c_str(),ios::app); //to append
  if(!ofile)
  {
    cout<<"Can't open "<<fname<<" for writing.\n";
    exit(0);
  }
  ofile<<"\n\nThe Mood & Brown chi square statistic Chi^2= ";
  ofile<<setprecision(5)<<Chi2<<"\n";
  ofile<<"Equivalently, V= M[1]^2/n[1]+...+M[K]^2/n[k]=";
  ofile<<setprecision(5)<<V0<<" \n \n";
  ofile<<setprecision(5)<<"The P-value P[V>="<<V0<<"]= ";
  ofile<<setprecision(12)<<A[K].Qk<<"\n";
```

```
  ofile<<"for K="<<K<<", n=(";
  for( i=1; i<K; i++) ofile<<n[i]<<", ";
  ofile<<n[K]<<"), and  a="<<a<<".\n";
  ofile<<"count= "<<counts<<"\n";
  ofile.close();
}

void contrasts()
{
  int i;
  bool yes, ok;
  char ch;
  double phi, Cbar, prob, var;
  double* C=new double[K+1];
  do
  {
    start: cout<<"Do you wish to enter a contrast?\n";
    do
    {
      cout<<"Please enter y)es or n)o ";
      cin>>ch;
      yes=(ch=='y')||(ch=='Y');
      ok=yes||(ch=='n')||(ch=='N');
    } while (!ok);
    if(yes)
    {
      cout<<"The values of M[i]-a*n[i]/N are :\n";
      for(i=1; i<=K; i++)
        cout<<setw(7)<<setprecision(4)<<dm[i]-dn[i]*a/dN[K]<<" ";
      cout<<"\n";
      phi=0; Cbar=0;
      cout<<"\nEnter "<<K<<" constants that add to zero :\n";
      for(i=1; i<=K; i++) cin>>C[i];
      for(i=1; i<=K; i++) Cbar+=C[i];
      Cbar/=(double)K;
      for(i=1; i<=K; i++) C[i]-=Cbar; //replace C[i] by C[i]-Cbar
      for(i=1; i<=K; i++) phi+=(C[i]*m[i])/dn[i];
      cout<<"phi= "<<phi<<"\n";
```

```
      var=Vstat(K,C,n);
      if(var>0) V0=sqr(phi)/var+sqr(da)/dN[K];
      else
      {
        cout<<"All zero contrast, start over:\n";
        goto start;
      }
      setStartA();
      setProb();
      prob=1.0-A[K].Qk;
      cout<<"Confidence probability for this contrast is : ";
      cout<<setprecision(6)<<prob<<"\n";
      if(writeFile)
      {
        ofile.open(fname.c_str(),ios::app);
        if(!ofile)
        {
          cout<<"Can't open "<<fname<<" for writing.\n";
          exit(0);
        }
        ofile<<"\n\nContrast Coefficients C=(";
        for(i=1; i<K; i++) ofile<<C[i]<<", ";
        ofile<<C[K]<<").\n";
        ofile<<"Value of contrast ";
        ofile<<"C[1]m[1]/n[1]+...+C[K]m[k]/n[K]=";
ofile<<setprecision(5)<<phi;
        ofile<<"\nConfidence probability : ";
ofile<<setprecision(5)<<prob<<" \n\n";
        ofile.close();
      }
    }
    else delete[] C;
  } while(yes);
}

void outputAnswers()
{
  printAnswers();
```

```
  if(writeFile) writeAnswer();
}

void PrintProgramTime(time_t startT, time_t endT,
 clock_t startC,clock_t endC)
{
  cout<<"Program time : "<<difftime(endT,startT)<<" seconds.\n";
  cout<<"Program ticks: "<<endC-startC<<" ticks.\n";
}

int main()
{
  getInput();
  Allocate();
  initialize();
  printInput();
  setStats();
  startTime=time(NULL);
  startTick=clock();
  setStartA();
  setProb();
  outputAnswers();
  endTime=time(NULL);
  endTick=clock();
  PrintProgramTime(startTime,endTime, startTick, endTick);
  contrasts();
  DeAllocate();
  return 1;
}
```

Appendix O

C++ program to calculate the P-value for the H test.

```
//HTest.cpp . C++ program to calculate the exact P-value of the Kruskal
//Wallis H test for a small matrix of counts using a convolution.
//Copyright (C) 2001, Jerome Klotz and Hongsuk Jorn
//University of Wisconsin and Inha University
#include <iostream>
#include <math.h>
#include <float.h>
#include <iomanip>
#include <ctime>
#define min(a,b) (((a)<(b))? (a):(b))
using namespace std;

//global values
int K, C;   //K rows, C columns in count matrix
int N;   //Total counts
int cnt=0;  //number of nodes set
int *n,*t,*u; //n[i] is ith sample size ,t[j] ties, u row of matrix
int **U0;     //U0[i][j] is data matrix of counts
double *a;    //(a[1],a[2],...,a[C]) are average ranks
double H0, V0;//statistics for data
double *lnFac;//lnFac[m]=log(m!)
time_t  startTime, endTime;//for timing the calculation in seconds
clock_t startTick, endTick;//for timing clock ticks of the computer
```

```
class node
{//a node has {v,p,(t[1],t[2],...,t[C]),(u[1].u[2],...,u[C])}
public:
  double v,p;//node double values
  int *t, *u;//node vector values

  node(double v0=0, double p0=0, int *t0=NULL, int *u0=NULL)
  {//for constructing a node from values (v0,p0,t0,u0)
    v=v0; p=p0;
    if(t0!=NULL)
    {
      t=new int[C+1];
      for(int j=1; j<=C; j++) t[j]=t0[j];
    }
    else t=NULL;
    if(u0!=NULL)
    {
      u=new int[C+1];
      for(int j=1; j<=C; j++) u[j]=u0[j];
    }
    else u=NULL;
  }

  node& node::operator=(const node &r)
  {//to set one node = another
    int j;
    if(&r!=this)
    {
      v=r.v;
      p=r.p;
      delete[] t;
      t=new int[C+1];
      for(j=1; j<=C; j++) t[j]=r.t[j];
      delete[] u;
      u=new int[C+1];
      for(j=1; j<=C; j++) u[j]=r.u[j];
```

```
    }
    return *this;
  }

    ~node()
    {//for deleting a node
      delete[] t;
      delete[] u;
    }
} *Array;//for Array[1,...,K] of nodes

void PrintHeading()
{
  cout<<"Exact P-value for the Kruskal-wallis H test with ties\n";
  cout<<"Program for small arrays of counts.\n";
  cout<<"Copyright (C) Jerome Klotz and Hongsuk Jorn\n";
  cout<<"University of Wisconsin and Inha University.\n";
}

void SetKC()
{//sets dimensions of count matrix
 cout<<"\nEnter number of rows K    : ";
 cin>>K;
 cout<<  "Enter number of columns C : ";
 cin>>C;
}

void Allocate()
{//allocates storage depending on K,C
  U0=new int*[K+1];
  for(int i=0; i<=K; i++) U0[i]=new int[C+1];
  n=new int[K+1];
  t=new int[C+1];
  u=new int[C+1];
  a=new double[C+1];
  Array=new node[K+1];//allocate space (array of default nodes)
}
```

```
void DeAllocate()
{//deletes vectors to free storage when finished
  for(int i=0; i<=K; i++) delete [] U0[i];
  delete [] U0;  delete [] n;  delete [] t;
  delete [] u;   delete [] a;  delete [] lnFac;
  delete [] Array;
}

void SetCounts()
{//gets initial count matrix
  int i,j;
  cout<<"Enter counts by rows ("<<K<<" rows, "<<C<<" columns):\n";
  for(i=1; i<=K; i++)
  {
    cout<<"Enter U["<<i<<"]: ";
    for(j=1; j<=C; j++) cin>>U0[i][j];
  }
  cout<<"\n";
}

void SetMargins()
{//sets margins, & N from initial count matrix
  int i,j;
  N=0;
  for(i=1; i<=K; i++)//row margins
  {
    n[i]=0;
    for(j=1;j<=C; j++) n[i]+=U0[i][j];
    N+=n[i];
  }
  for(j=1; j<=C; j++)//column margins
  {
    t[j]=0;
    for(i=1; i<=K; i++) t[j]+=U0[i][j];
  }
}
```

```
void PrintCounts(int **U)
{//prints array (U[i,j]) and margin totals
  int i,j;
  cout<<"\n"<<K<<"x"<<C<<" Data Matrix & Margins\n";
  for(i=1; i<=K; i++)
  {
    cout<<"|";
    for (j=1; j<=C; j++)
    {
     cout.width(4);
     cout<<U[i][j]<<" ";
    }
    cout<<"|";
    cout.width(4);
    cout<<n[i]<<"\n";
  }
  cout<<"_";
  for(j=1; j<=C; j++)
  {
    cout<<"_____";
  }
  cout<<"______\n"<<"|";
  for(j=1; j<=C; j++)
  {
    cout.width(4);
    cout<<t[j]<<" ";
  }
  cout<<"|";
  cout.width(4);
  cout<<N<<"\n\n";
}

void SetLnFac()
{//sets log(m!) for m=0,1,...,N
  int i;
  double sum=0;
  lnFac=new double[N+1];
  lnFac[0]=lnFac[1]=0;
```

```
  for(i=2; i<=N; i++)
  {
    sum+=log((double)i);
    lnFac[i]=sum;
  }
}

void SetStartVec(int* u, const int ni , const int* t)
{//sets a lexical "smallest" single vector (u[1],...,u[C]),
 //so that 0<=u[i]<=t[i] and u[1]+...+u[C]=ni
  int i,sum=ni;
  for(i=1; i<=C; i++)
  {
    u[i]=min(sum,t[i]);
    sum-=u[i];
  }
}

bool NextVec(int* u, int ni, int* t)
{//if possible, changes vector (u[1],u[2],...,u[C]) to next "largest"
 //vector and returns true. Otherwise returns false if vector is
 //already "largest" and vector remains unchanged.
  int i=0,j,sum=-1;
  bool cellfull;
  do i++; while(u[i]==0);//skip initial zeros
  if(i==C) return false; //trivial case of all zeros
  do
  {
    sum+=u[i];
    i++;
    cellfull=(u[i]==min(ni,t[i]));
  } while(cellfull &&(i<C));//i is index of first non full cell
  if(cellfull) return false;//already "largest" case (no change)
  u[i]++;
  for(j=1; j<i; j++)
  {
    u[j]=min(sum,t[j]);
    sum-=u[j];
```

```
  }
  return true;//(u[1],u[2],...,u[C]) changed to next "largest"
}

void SetRanks()
{//sets average rank values in (a[1],a[2],...,a[C])
  int j;
  a[1]=((double)(t[1]+1))/2.0;
  for(j=2; j<=C; j++)
  a[j]=a[j-1]+((double)(t[j-1]+t[j]))/2.0;
}

double Statistic(int **U)
{//calculates V for the KxC array (U[i,j])
  int i,j;
  double R,V=0;
  for(i=1; i<=K; i++)
  {
    R=0;
    for(j=1; j<=C; j++) R+=a[j]*((double)U[i][j]);
    V+=R*R/((double)n[i]);
  }
  return V;
}

double HStatistic(double V)
{//calculates H test statistic using V
  int j;
  double H, dN=(double)N, dt, dC=dN*(dN+1.0);
  double gamma=0;//tie correction factor
  for(j=1; j<=C; j++)
  {
    dt=(double)t[j];
    gamma+=(dt+1)*dt*(dt-1);
  }
  H=(12.0/( dC*(1-gamma/(dC*(dN-1))) ))*(V-dC*(dN+1)/4.0);
  return H;
}
```

```
void SetH0_V0()
{//sets H and V for the data
  V0=Statistic(U0);
  H0=HStatistic(V0);
}

void PrintH0_V0()
{//prints H and V for the data
  cout<<"\nTest statistics using average ranks:\n";
  cout<<"Kruskal Wallis statistic with ties H="<<H0<<"\n";
  cout<<"  R[1,+]^2/n[1]+...+R[K,+]^2/n[K]= V="<<V0<<"\n\n";
}
void PrintRanks()
{//prints average ranks a[j], j=1,2,...,C
  int j;
  cout<<"Average Ranks:\n";
  for(j=1; j<=C; j++) cout<<a[j]<<" ";
  cout<<"\n";
}

void SetStartArray()
{//sets initial Array[1,2,...,K] of nodes starting at K
  int i,j;
  double v,R;
  int *t0=new int[C+1];
  v=V0;
  for(j=1; j<=C; j++) t0[j]=t[j];
  SetStartVec(u,n[K],t0);
  Array[K]=*new node(v,0,t0,u);
  for(i=K-1; i>0; i--)
  {
    R=0;
    for(j=1; j<=C; j++)
    {
      R+=a[j]*Array[i+1].u[j];
      t0[j]-=Array[i+1].u[j];
    }
```

```
    v-=R*R/((double)n[i+1]);
    SetStartVec(u,n[i],t0);
    Array[i]=*new node(v,0,t0,u);
  }
}

void ResetArray(int k)
{//resets Array[k,k-1,...,1] using Array[k+1]
  int i,j;
  double R;
  for(i=k; i>0; i--)
  {
    R=0;
    for(j=1; j<=C; j++)
    {
      Array[i].t[j]=Array[i+1].t[j]-Array[i+1].u[j];
      R+=(Array[i+1].u[j])*a[j];
    }
    Array[i].v=Array[i+1].v-R*R/((double)n[i+1]);
    Array[i].p=0;
    SetStartVec(Array[i].u,n[i],Array[i].t);//set u vector
  }
}

void PrintArray()
{//prints Array[1,2,...,K] for checking
  int i,j;
  for(i=1; i<=K; i++)
  {
    cout<<"i="<<i<<", ("<<Array[i].v<<", "<<Array[i].p<<", t=(";
    for(j=1; j<=C; j++) cout<<Array[i].t[j]<<", ";
    cout<<"),  u=(";
    for(j=1; j<=C; j++) cout<<Array[i].u[j]<<", ";
    cout<<").\n";
  }
}
```

```
double Prob(int *u, int *t)
{//calculates binomial (product{ t[j]_C_u[j]: j=1,2,...,C })/(N0_C_n0)
 //using log factorials where N0=t[1]+t[2]+...t[C], n0=u[1]+...+u[C]
  int j,n0=0,N0=0;
  double lnP=0;
  for(j=1; j<=C; j++)
  {
    lnP+=(lnFac[t[j]]-lnFac[u[j]]-lnFac[t[j]-u[j]]);
    N0+=t[j]; n0+=u[j];
  }
  lnP-=(lnFac[N0]-lnFac[n0]-lnFac[N0-n0]);
  return exp(lnP);
}

void SetProb()
{//sets probabilities for k=1,2,...,K
  double V1,R1,epsilon=1.0e-8;
  bool done;
  int i=1,j;
  do
  {
    if(i==1)
    {
      R1=0;
      for(j=1; j<=C; j++) R1+=Array[1].u[j]*a[j];
      V1=R1*R1/((double)n[1]);
      if(V1>=Array[1].v-epsilon) Array[1].p=1;
      else Array[1].p=0;
      i++; cnt++;
    }
    else
    {
      Array[i].p+=Array[i-1].p*Prob(Array[i].u,Array[i].t);
      done=!NextVec(Array[i].u,n[i],Array[i].t);//try to change u
      if(!done) //reset lower array if changed
      {
        ResetArray(i-1);//from i-1 downto 1
        i=1;//now start at 1 and build up
```

```
      }
      else i++;//go up one stage and add lower stage prob.
    }
  } while (i<=K);
}

void PrintProb()
{
  cout<<"\nP-value:\n";
  cout<<"P[ H>="<<H0<<" |t]= "<<Array[K].p<<"\n";
  cout<<"\nNode count="<<cnt<<".\n\n";
}

void PrintProgramTime(time_t startT, time_t endT, clock_t startC,clock_t endC)
{
  cout<<"Program time : "<<difftime(endT,startT)<<" seconds.\n";
  cout<<"Program ticks: "<<endC-startC<<" ticks.\n";
}

int main()
{
  PrintHeading();
  SetKC();
  Allocate();
  SetCounts();
  SetMargins();
  PrintCounts(U0);
  startTime=time(NULL);
  startTick=clock();
  SetRanks();
  PrintRanks();
  SetLnFac();
  SetH0_V0();
  PrintH0_V0();
  SetStartArray();
  SetProb();
  PrintProb();
  endTime=time(NULL);
```

```
  endTick=clock();
  PrintProgramTime(startTime,endTime, startTick, endTick);
  DeAllocate();
  return 1;
}
```

Appendix P

C++ P-value program for the Benard van Elteren test.

```
//BenVanElt.cpp Benard-van Elteren test calculation.
#include <iostream>
#include <fstream>
#include <stdlib.h>
#include <cmath>
#include <vector>
#include <list>
#include <iterator>
#include <algorithm>
#include <iomanip>
#include "cdf.h"
using namespace std;

class Dta
{
  public:
   int i;             //row index
   double Xijk, Rijk; // data values and ranks
   Dta(int c=0, double d=0, double e=0): i(c),Xijk(d),Rijk(e){}
   bool operator == (const Dta &y) const { return Xijk==y.Xijk; }
   bool operator < (const Dta &y) const {return Xijk<y.Xijk;}//sorts Xijk
};
bool sorti(const Dta &x, const Dta &y) { return x.i<y.i; }//to sort i
```

```
vector<Dta> *Block; //for Block[j].i and Blocj[j].Xijk values
vector<int> *t;     //for t[j][r] values, r=1,2,...,c[j]
vector<double> *a;  //a[j][r] is the average rank
int *c;             //for c[j] counts
int **n;            //for n[i][j] values
int *n_2;           //for n+j=n_2[j] values
double *gam;        //for gamma[j] values
int i,i1,i2,j,k,r;  //indices i,i1 rows, i2,j columns, k,r sum indices
int K,b;            //number of treatments, blocks
double **sigma11;   //for (sigma11[i1][12]:i1,i2=1,2,...K-1) matrix
double **L;         //lower triangular matrix for Sigma11=LL'
double *R;          //for (R1++,R2++,...RK++)
double *U;          //for (U[1],U[2],...,U[K])
double *ER;         //for (E(R[1]),E(R[2]),...,E(R[K]))
double *W;          //for quadratic form
double V;           //value of U'(Inveres(Sigma11)U
double alpha;       //P-value
ifstream infile;    //file for data

void PrintHeading(void)
{
  cout<<"\n\nBenard van Elteren test program by Jerome Klotz.\n";
  cout<<"It generalizes the Friedman, Cochran, and ";
  cout<<"Durban two way rank tests.\n\n";
}

void OpenDataFile(char *filename)
{
  infile.open(filename);
  if(!infile)
  {
    cout<<"Cannot open for input the file named \n"<<filename;
    cout<<"\n\n";
    exit(0);
  }
}
```

```
void GetKb(void)
{
  infile>>K>>b;
  if((K<2)||(b<1))
  {
    cout<<"Data too small, exit\n"; exit(0);
  }
}

void SetStorage(void)
{
  Block=new vector<Dta>[b+1];
  t=new vector<int>[b+1];
  a=new vector<double>[b+1];
  c=new int[b+1];
  n=new (int*)[K+1];
  for(i=1; i<=K; i++) n[i]=new int[b+1];
  n_2=new int[b+1];
  gam=new double[b+1];
  sigma11=new (double*)[K];
  for(i=1; i<K; i++) sigma11[i]=new double[K];
  L=new (double*)[K];
  for(i=1; i<K; i++) L[i]=new double[i+1]; //Lower triangular
  W=new double[K];
  R=new double[K+1];
  U=new double[K+1];
  ER=new double[K+1];
}

void Get_nij()
{
  for(i=1; i<=K; i++) for(j=1; j<=b; j++) infile>>n[i][j];
  for(j=1; j<=b; j++)
  {
    n_2[j]=0;
    for(i=1; i<=K; i++) n_2[j]+=n[i][j];
  }
}
```

```
void Print_nij(void)
{
  cout<<"Cell counts n[i,j] for treatment row i=1,..,"<<K;
  cout<<", and block j=1,..,"<<b<<" .\n";
  cout<<setfill('_')<<setw(5*b+7)<<"_"<<"\n"<<setfill(' ');
  for(i=1; i<=K; i++)
  {
    cout<<"       ";
    for(j=1; j<=b; j++)  cout<<setw(5)<<n[i][j];
    cout<<"\n";
  }
  cout<<setfill('_')<<setw(5*b+7)<<"_"<<"\n"<<setfill(' ')<<"n[+,j] ";
  for(j=1; j<=b; j++) cout<<setw(5)<<n_2[j];
  cout<<"\n\n";
}

void GetXijk(void)
{
  Dta Value;          //for setting up data structure
  double Xijk;
  for(i=1; i<=K; i++) for(j=1; j<=b; j++) for(k=1; k<=n[i][j]; k++)
  {
    infile>>Xijk;
    Value.Xijk=Xijk; Value.i=i; Block[j].push_back(Value);
  }
}

void CloseDataFile(void)
{
  infile.close();
}

void Set_tj_aj_gamj(void)
//for ties, average ranks, and tie correction
{
  vector<Dta>::iterator itd, itd1, itd2;
  vector<int>::iterator itr;
```

```
  vector<double>::iterator ita;
  for(j=1; j<=b; j++)
  {
    sort(Block[j].begin(),Block[j].end()); //sorts Block[j] on Xijk
    a[j].push_back(1); t[j].push_back(0); t[j].push_back(1);
    i=1; r=1;
    itd2=Block[j].end(); itd2--;
    for(itd=Block[j].begin(); itd!=itd2; itd++) //set t[j][r] values
    {
      itd1=itd; itd1++;
      if((itd->Xijk)==(itd1->Xijk)) t[j][r]++;
      else { r++; t[j].push_back(1);}
    }
    c[j]=t[j].size()-1;
    for(r=1; r<=c[j]; r++)
    //set integer a[j]=2*(j-th largest average rank value)
      a[j].push_back(a[j][r-1]+t[j][r-1]+t[j][r]);
    gam[j]=0;
    for(r=1; r<=c[j]; r++) //set gam[j] values
      gam[j]+=(double)((t[j][r]-1)*t[j][r]*(t[j][r]+1));
  }
}

void SetRijk()
{
  vector<Dta>::iterator itd;
  for(j=1; j<=b; j++)
  {
    k=1; r=1;
    for(itd=Block[j].begin(); itd!=Block[j].end(); itd++)
    //set Rijk values to ave. ranks
    {
      itd->Rijk=a[j][r]/2.0; k++;
      if(k>t[j][r]){ k=1; r++; }
    }
  }
}
```

```
void SetU(void)
{
  vector<Dta>::iterator itd;
  for(j=1; j<=b; j++) sort(Block[j].begin(),Block[j].end(),sorti);
  //sorts on i
  for(i=1; i<=K; i++)
  {
    R[i]=0; ER[i]=0;
    for(j=1; j<=b; j++)
    {
      ER[i]+=n[i][j]*(n_2[j]+1.0)/2.0;
      for(itd=Block[j].begin(); itd!=Block[j].end(); itd++)
        if(itd->i==i) R[i]+=itd->Rijk;
    }
    U[i]=R[i]-ER[i];
  }
}

void SetSigma11(void)
{
  vector<Dta>::iterator itd;
  double Const;
  for(i1=1; i1<K; i1++)
   for(i2=1; i2<K; i2++)
   {
     sigma11[i1][i2]=0;
     for(j=1; j<=b; j++)
     {
       Const=( 1.0-gam[j]/((n_2[j]-1.0)*n_2[j]*(n_2[j]+1.0)) )/12.0;
       if(i1==i2) sigma11[i1][i1]+=
                    n[i1][j]*(n_2[j]-n[i1][j])*(n_2[j]+1.0)*Const;
       else sigma11[i1][i2]-=n[i1][j]*n[i2][j]*(n_2[j]+1.0)*Const;
     }
   }
}

void SetCholeski(void) //Sets lower triangular Choleski factor L
{       // where Sigma11=LL' is positive definite, symmetric.
```

```
  const double epsilon=1.0E-10; //for singularity test.
  double sum, lamMin=1.0E25, lamMax=0;
  for(i1=1; i1<=K-1; i1++)
    for(i2=1; i2<=i1; i2++)
    {
      sum=0;;
      L[i1][i2]=sigma11[i1][i2];
      for(k=1; k<i2; k++)
        sum+=L[i1][k]*L[i2][k];
      L[i1][i2]-=sum;
      if(i1==i2)
      {
        lamMin=min(L[i1][i1],lamMin);
        lamMax=max(L[i1][i1],lamMax);
        if((lamMax<epsilon)||(lamMin/lamMax)<epsilon)
        {
          cout<<"Singular covariance matrix. Incorrect design.";
          cout<<"Program exit.\n\n";  exit(0);
        }
        L[i1][i1]=sqrt(L[i1][i1]);
      }
      else L[i1][i2]/=L[i2][i2];
    }
}

void PrintCholeski(void)
{
  cout<<"\n\nL[i1,i2] :\n";
  for(i1=1; i1<K; i1++)
  {
    for(i2=1; i2<=i1; i2++) cout<<L[i1][i2]<<", ";
    cout<<"\n";
  }
  cout<<"\n\n";
}

void SetQuadForm()
{
```

```
  double sum;
  for(i1=1; i1<K; i1++)
  {
    sum=0;
    for(k=1; k<i1; k++) sum+=L[i1][k]*W[k];
    W[i1]=(U[i1]-sum)/L[i1][i1];
    V+=sqr(W[i1]);
  }
}

void PrintSigma11(void)
{
  cout<<"Sigma11[i1,i2] for i1,i2=1,..,K-1="<<K-1<<"\n";
  for(i1=1; i1<K; i1++)
  {
    for(i2=1; i2<K; i2++)
    {
      cout<<sigma11[i1][i2];
      if(i2<K-1) cout<<", ";
    }
    cout<<"\n";
  }
  cout<<"\n\n";
}

void PrintData(void)
{
  vector<Dta>::iterator itd;
  cout<<"Average ranks:(a[j,r] : r=1,..,c[j]), j=1,..,"<<b<<"\n";
  cout<<setfill('_')<<setw(47)<<"_"<<"\n"<<setfill(' ');
  for(j=1; j<=b; j++)
  {
    cout<<"(";
    for(r=1; r<=c[j]; r++)
    {
      cout<<a[j][r]/2.0;
      if (r==c[j]) cout<<")";
      else cout<<", ";
```

```
    if(j<b) cout<<", ";
    else cout<<" ";
  }
  if(j%6==0) cout<<"\n  ";
}
cout<<"\n\n";
cout<<"Values of (R[i++],E(R[i++]),R[i++]-E(R[i++])) for i=1,..,"<<K<<".\n";
cout<<setfill('_')<<setw(58)<<"_"<<"\n"<<setfill(' ');
for(k=1; k<=3; k++)
{
  switch(k)
  {
    case 1: cout<<"R[i++]           "; break;
    case 2: cout<<"E(R[i++])        "; break;
    case 3: cout<<"R[i++]-E(R[i++]) "; break;
  }
  switch(k)
  {
    case 1: for(i=1; i<=K; i++) cout<<setw(7)<<R[i]<< "  "; break;
    case 2: for(i=1; i<=K; i++) cout<<setw(7)<<ER[i]<<"  "; break;
    case 3: for(i=1; i<=K; i++) cout<<setw(7)<<U[i]<< "  "; break;
  }
  cout<<"\n";
}
cout<<"\n\n";
cout<<"Row :{(Xijk, Rijk):k=1,..,n[ij]},i=1,..,"<<K<<", j=1,..,"<<b<<".\n";
cout<<setfill('_')<<setw(52)<<"_"<<"\n"<<setfill(' ');
for(i=1; i<=K; i++)
{
  cout<<i<<":   "; r=0;
  for(j=1; j<=b; j++)
  {
     k=0;
     for(itd=Block[j].begin(); itd!=Block[j].end(); itd++)
     {
       if((k==0)&&(itd==Block[j].begin()))
       {
         cout<<"{";
```

```
          if(n[i][j]==0) cout<<((j<b)?"}, ":"}  ");
        }
        if(itd->i==i)
        {
          k++;
          cout<<"("<<itd->Xijk<<", "<<itd->Rijk<<")";
          if(k<n[i][j]) cout<<", ";
          else
            if(j<b) cout<<"},  ";
            else  cout<<"}  ";
          if((r+1)%6==0) cout<<"\n      "; r++;
        }
      }
    }
    cout<<"\n";
  }
  cout<<"\n\n";
}

void SetAlpha(void)
{
  alpha=1.0- cdf::icgamma(V/2.0, (K-1)/2.0);
}

void PrintAnswers()
{
  cout<<"Value of Benard van Elteren statistic V= "<<V<<" .\n\n";
  cout<<"P-value by a central Chi-square approximation ";
  cout<<"with K-1="<<K-1<<" degrees of freedom:\n\n";
  cout<<"          P[ChiSquare("<<K-1<<")>"<<V<<"]="<<alpha<<".\n\n";
}

void CleanUp(void)
{
  delete[] Block;     delete[] t;
  delete[] a; delete[] c;
  for(i=0; i<=K; i++) delete[] n[i];
  delete[] n;         delete[] n_2;
```

```
  delete[] gam;
  for(i=1; i<K; i++)  delete[] sigma11[i];
  delete[] sigma11;
  for(i=1; i<K; i++)  delete[] L[i];
  delete[] L;
  delete[] U;         delete[] W;
  delete[] R;         delete[] ER;
}

int main(int argc, char *argv[])
{
  PrintHeading();
  OpenDataFile(argv[1]);
  GetKb();
  SetStorage();
  Get_nij();
  Print_nij();
  GetXijk();
  CloseDataFile();
  Set_tj_aj_gamj();
  SetRijk();
  SetU();
  SetSigma11();
  SetCholeski();
  SetQuadForm();
  PrintData();
  SetAlpha();
  PrintAnswers();
  CleanUp();
  return(1);
}
```

Appendix Q

C++ program for exact and approximate P-values for Friedman's test with ties.

```
#include <iostream>
#include <string>
#include <fstream>
#include <iomanip>
#include <vector>
#include <algorithm>
#include "cdf.h" //includes #define sqr(a) ((a)*(a)) and icbeta for chi sq

using namespace std;

float **X,Q,alpha,g0, *gammaj; //Xij values, Statistic, tie factor,
int K,b,*c; //number of rows, columns, ties
long countN,countD,Kfac; //numerator, denometer counts, K!
long *cnt,*PermLim; // permutation count and total for column R[j]
vector<int> *t;

class Dta
{
       public:
int i;
float Xij, Rij;
```

```
~Dta(){}
Dta &operator=(const Dta &r)
{
if (&r!=this) { i=r.i; Xij=r.Xij; Rij=r.Rij;}
return *this;
}
        bool operator == (const Dta &y) const {return Xij==y.Xij;}
bool operator < (const Dta &y) const {return Xij<y.Xij;} //for sorting Xij
};
bool sorti(const Dta &x, const Dta &y) { return x.i<y.i;} //for sorting i

vector<Dta> *Block; //for Block[j].i, Block[j].Xij, Block[j].Rij
vector<float> *R;

void GetFileData() //Sets storage also
{
int i,j;
string filename;
cout<<"\nEnter input data file name: ";
cin>>filename;
ifstream infile(filename.c_str());
if(!infile)
{
cout<<"Cannot open input file "<<filename<<"\n";
exit(0);
}
infile>>K>>b;
X=new float *[K];
for(i=0; i<K; i++) X[i]=new float[b];
for(i=0; i<K; i++) for(j=0; j<b; j++) infile>>X[i][j];
infile.close();
cnt=new long[b-1];
c=new int[b];
PermLim=new long[b-1];
Block=new vector<Dta>[b];
R=new vector<float>[b];
gammaj=new float[b];
t=new vector<int>[b];
```

```
}

long Factorial(int n) //calculates n!
{
long fac=1, nL=(long)n;
for(long r=2; r<=nL; r++) fac*=r;
return fac;
}

long Multinomial(long n, vector<int>s)
{
long denom=1;
for(int r=0; r<s.size(); r++) denom*=Factorial(s[r]);
return Factorial(n)/denom;
}

void PrintX() //Prints X matrix and sets K!
{
int i,j;
cout<<"Input Data X[i,j] for i="<<"1,2,...,"<<K;
cout<<" (treatments), j=1,2,...,"<<b<<" (blocks).\n";
for(i=0; i<K; i++)
for(j=0; j<b; j++)
   cout<<setw(6)<<X[i][j]<<((j<(b-1))? " ":"\n");
cout<<"\n";
Kfac=Factorial(K); //sets K!
}

void SetBlocks(void) //Sets Block[j], j=0,1,...,b-1
{
int i,j,k,r;
vector<float>a;
vector<int> t;
int ct;
        Dta Z;
vector<Dta>::iterator itd,itd1,itd2;
for(j=0; j<b; j++)
{
```

```
k=1;
a.push_back(1);
t.push_back(0);
t.push_back(1);
for(i=0; i<K; i++)
{
Z.i=i; Z.Xij=X[i][j]; Z.Rij=0;
Block[j].push_back(Z);
                }
sort(Block[j].begin(), Block[j].end());
itd2=Block[j].end(); itd2--;
                for(itd=Block[j].begin(); itd!=itd2; itd++)
{
itd1=itd; itd1++;
if((itd->Xij)==(itd1->Xij)) t[k]++;
else { k++; t.push_back(1);}
}
ct=t.size()-1;
for(r=1; r<=ct; r++) a.push_back(a[r-1]+t[r-1]+t[r]);
k=1; r=1;
for(itd=Block[j].begin(); itd!=Block[j].end(); itd++)
{
itd->Rij=a[r]/2.0; k++;
if(k>t[r]) { k=1; r++; }
}
a.erase(a.begin(),a.end()); t.erase(t.begin(),t.end());
sort(Block[j].begin(), Block[j].end(),sorti);
       }
}


void PrintBlocks() //Prints Blocks
{
int i=0,j;
cout<<"\n";
vector<Dta>::iterator itd;
for(j=0;j<b; j++)
{
```

```
          {
           for(itd=Block[j].begin(); itd<Block[j].end(); itd++)
     cout<<setw(6)<<itd->i<<" "<<setw(6)<<itd->Xij<<" "<<setw(6)<<itd->Rij<<"\n";
   cout<<"____________________\n";
  }
  i++;
}

}

void SetR() //Sets R matrix
{
int j;
vector<Dta>::iterator itd;
for(j=0; j<b; j++)
 for(itd=Block[j].begin(); itd!=Block[j].end(); itd++)
           R[j].push_back(itd->Rij);
}

void PrintR() //Prints R matrix
{
int i,j,r;
float SumRj;
cout<<"Average Ranks R[i,j]";
cout<<setw(6+((b-1)*7)-19)<<" "<<"| R[i+]\n";
for(i=0; i<K; i++)
{
SumRj=0;
for(r=0; r<b; r++) SumRj+=R[r][i];
for(j=0; j<b; j++)
{
cout<<setw(6)<<R[j][i]<<" ";
}
cout<<"| "<<SumRj<<"\n";
}
cout<<"\n";
}
```

```
float FriedStat() //calculates Friedman statistic with tie factor
{
int i,j,r;
float V,W;
vector<Dta>::iterator itd,itd1,itd2;
W=0; //compute  sum{ sum(R[i,j]-b(K+1)/2) : 0<=j<K }^2 : 0<=i<b}
for(i=0; i<K; i++)
{
V=0;
for(j=0; j<b; j++) V+=R[j][i];
V-=((float)(b*(K+1)))/2.0;
W+=sqr(V);
}
g0=0; //now compute tie correction g0=sum(gamma[j])
for(j=0; j<b; j++) //set t[j][r], PermLim[j], and get gamma
{
sort(Block[j].begin(),Block[j].end());
t[j].push_back(1);
r=0;
itd2=Block[j].end(); itd2--;
for(itd=Block[j].begin(); itd!=itd2; itd++)
{
itd1=itd; itd1++;
if((itd->Xij)==(itd1->Xij)) t[j][r]++;
else { r++; t[j].push_back(1);}
}
c[j]=t[j].size();
gammaj[j]=0;
for(r=0; r<c[j]; r++)
  gammaj[j]+=(float)(t[j][r]-1)*t[j][r]*(t[j][r]+1);
g0+=gammaj[j];
PermLim[j]=Multinomial(K,t[j]);
}
W*=12.0/(((float)b*K*(K+1))*(1.0-g0/((float)b*(K+1)*K*(K-1))));
return W;
}

float Statistic() //Calculate statistic  sum{ sum(R[i,j] : 0<=j<K }^2 : 0<=i<b
```

```
{
int i,j;
float V,stat=0;
for(i=0; i<K; i++)
{
V=0;
for(j=0; j<b; j++) V+=R[j][i];
stat+=sqr(V);
}
return stat;
}

double GetPvalue()
{
float epsilon=1.0E-3;
int r,k,s;
        countN=0; countD=0;
for(r=0; r<(b-1); r++) { cnt[r]=0;}
do //while k<(b-1)
{
k=0;
while (cnt[k]<PermLim[k])
{
next_permutation(R[k].begin(),R[k].end());
if(Statistic()>(Q-epsilon)) countN++; countD++;
cnt[k]++;
};
           A0:  k++;
cnt[k]++;
if(k<(b-1)) if(cnt[k]<PermLim[k])
    {
     for(r=0; r<k; r++) cnt[r]=0;
               next_permutation(R[k].begin(),R[k].end());
    }
    else { goto A0;}
} while(k<(b-1));
alpha=((double)countN)/((double)countD);
return alpha;
```

```
}

void PrintPvalue()
{
long no=1; int j,r;
float W=FriedStat();
cout<<"Friedman statistic (corrected for ties) :"<<W<<"\n";
cout<<"Tie correction factor gamma=sum(gamma[j]) :"<<g0<<"\n";
cout<<"Approximate P-value : P[Chi Square > "<<W<<" | "<<K-1;
cout<<" d.f. ]="<<1.0-cdf::icgamma(W/2.0,(K-1)/2.0)<<"\n";
for(j=0; j<(b-1); j++) no*=PermLim[j];
cout<<"\nPermuting Product{(K!)/(t[j][1]!...t[j][c[j]]!) :";
cout<<" j=1,...,b-1}="<<no<<" columns and calculating statistics.\n";
cout<<"If this number is large, it may take a while.\n\n";
cout<<"Tie counts {t[j][r] :r=1,2,...,c[j]} for columns 1,2";
if(b==3) cout<<",3 :";
if(b>3) cout<<",...,"<<b<<" :";
for(j=0; j<b; j++)
{
                if(j%8==0) cout<<"\n";
cout<<"(";
for(r=0; r<c[j]; r++)
{
cout<<t[j][r];
if(j<(b-1)) cout<<((r<(c[j]-1))?", ":"),");
else cout<<((r==(c[j]-1))?") ":", ");
}
}
cout<<".\n";
cout<<"Permutation counts for columns 1,2";
if(b==3) cout<<" : ";
if(b==4) cout<<",3 : ";
if(b>4) cout<<",...,"<<(b-1)<<" :";
cout<<"(";
for(j=0; j<(b-1); j++) cout<<PermLim[j]<<((j<(b-2))? ", ":") .\n");
alpha=GetPvalue();
cout<<"Equivalent Statistic Q="<<Q<<"\n";
cout<<"Exact P-value : "<<countN<<"/"<<countD<<"="<<alpha<<"\n";
```

```
}

void Heading()
{
cout<<"\nExact and approximate P-value for Friedman's test by Jerome Klotz.\n";
}

void CleanUp()
{
for(int i=0; i<K; i++) delete[]X[i];
delete[]X;
delete[]R;
delete[]cnt;
delete[]c;
delete[]PermLim;
delete[]gammaj;
delete[]t;
}

int main()
{
Heading();
GetFileData();
PrintX();
SetBlocks();
SetR();
PrintR();
Q=Statistic();
PrintPvalue();
CleanUp();
return 1;
}
```

Appendix R

P-values for Durban's nonparametric incomplete block test.

```
//Program to calculate the exact P-value for Durban's test.
#include <iostream>
#include <string>
#include <fstream>
#include <iomanip>
#include <vector>
#include <algorithm>
#include "cdf.h" //includes #define sqr(a) ((a)*(a)) and icbeta for chi sq

using namespace std;

const double epsilon=1.0E-10;
int **D, **n; //Balanced incomplete block treatments, value indicator
double **R; //Balanced incomplete block average ranks
int K,d,b; //dimensions: treatments, obs./block, blocks
double **Sigma, EV, *Ri, *U;
//Covariance, EV= E(R[i,+]), R[i,+], U[i]=R[i,+]-EV
double *W, **L, Q, sum; //U=LW, Sigma=LL', Q=W'W,
long countN, countD, *PermCount ,*t, *PermLim;
vector<int> gammaj; //tie factors: gamma[j]=(t[j]-1)*t[j]*(t[j]+1)
vector<double> *Z;
```

```
class Dta
{
public:
 int i;
         double Xij, Rij;
         bool operator == (const Dta &y) const {return Xij==y.Xij;}
 bool operator < (const Dta &y) const {return Xij<y.Xij;} //for sorting Xij
};
vector<Dta> s;

void Heading()
{
  cout<<"\nP-values for Durban's nonparametric balanced ";
  cout<<"incomplete block test by Jerome Klotz.\n\n";
}

long Factorial(int m)
{
  long fac=1, mL=(long)m;
  for(long i=2; i<=mL; i++) fac*=i;
  return fac;
}

long Multinomial(int N, vector<int> p)
{// calculates N!/(p[0]!p[1]!...p[k]!)
  long denom=1;;
  for(int i=0; i<p.size(); i++) denom*=Factorial(p[i]);
  return Factorial(N)/denom;
}


void GetDMatrix(char *filename)
{
  ifstream infile;
  infile.open(filename);
  if(!infile)
  {
```

```
    cout<<"Cannot open "<<filename<<" for input.\n";
    exit(0);
  }
  infile>>d>>b; //First line has row, column dimensions
  D=new int*[d];
  for(int i=0; i<d; i++) D[i]=new int[b];
  for(int i=0; i<d; i++) for(int j=0; j<b; j++) infile>>D[i][j];
  infile.close();
  K=0;
  for(int i=0; i<d; i++) for(int j=0; j<b; j++) K=max(K,D[i][j]);
}

void SetStorage()
{
  Z=new vector<double>[b];
  R=new double*[K+1];
  for(int i=0; i<=K; i++) R[i]=new double[b+1];
  n=new int*[K+1];
  for(int i=0; i<=K; i++) n[i]=new int[b+1];
  Sigma=new double*[K];
  for(int i=0; i<=K; i++) Sigma[i]=new double[K];
  L=new double*[K+1];
  for(int i=0; i<=K; i++) L[i]=new double[K+1];
  Ri=new double[K+1];
  U=new double[K+1];
  W=new double[K+1];
  PermCount=new long[b-1];
  PermLim=new long[b-1];
}

void PrintDMatrix()
{
    cout<<"Treatment matrix. Entries are treatments, columns are blocks.\n";
    for(int i=0; i<d; i++)
    {
      for(int j=0; j<b; j++) cout<<right<<setw(9)<<D[i][j]<<" ";
      cout<<"\n";
    }
```

```
}

void PrintZVector()
{
  cout<<"Value matrix. Entries are values, columns are blocks.\n";
  for(int i=0; i<d; i++)
  {
   for(int j=0; j<b; j++) cout<<right<<setw(9)<<Z[j][i]<<" ";
   cout<<"\n";
  }
}

void GetZMatrix(char *filename)
{
  double ZZ;
  ifstream infile;
  infile.open(filename);
  if(!infile)
  {
    cout<<"Cannot open "<<filename<<" for input.\n";
    exit(0);
  }
  for(int i=0; i<d; i++) for(int j=0; j<b; j++)
   { infile>>ZZ; Z[j].push_back(ZZ);}
  infile.close();
}

void SetRMatrix() //R[i,j] and tie factors gamma[j] using ties t
{
  Dta ss;
  vector<Dta>::iterator itd,itd1,itd2,itd3;
  vector<int> rr,t;
  int k,ct,e,h=1,jj=0,g0;
  vector<double> a;
  for(int i=1; i<=K; i++) for(int j=1; j<=b; j++) R[i][j]=0;
  for(int j=1; j<=b; j++)
  {
    k=1;
```

```
for(int i=1; i<=d; i++)
{
  int p=D[i-1][j-1];
  ss.i=p; ss.Xij=Z[j-1][i-1]; ss.Rij=0; s.push_back(ss);
}
sort(s.begin(),s.end());
a.push_back(1);  t.push_back(0), t.push_back(1);
itd2=s.end()-1;
for(itd=s.begin(); itd!=itd2; itd++)
 {
   itd1=itd; itd1++;
   if((itd->Xij)==(itd1->Xij)) t[k]++;
   else { k++; t.push_back(1); }
 }
g0=0;
for(h=1; h<t.size(); h++) g0+=(t[h]-1)*t[h]*(t[h]+1);
gammaj.push_back(g0);
ct=t.size();
for(e=1; e<ct; e++) a.push_back(a[e-1]+t[e-1]+t[e]);
k=1; e=1;
for(int i3=0; i3<ct; i3++)
{
  a[i3]=a[i3]/2.0; k++;
  if(k>t[e]) { k=1; e++;}
}
int c=1, g=1;
for(itd3=s.begin(); itd3!=s.end(); itd3++)
{
  if(c<=t[g]) { itd3->Rij=a[g]; c++;}
  else { c=1; g++; itd3->Rij=a[g]; c++;}
}
c=1;
for(itd3=s.begin(); itd3!=s.end(); itd3++)
for(int i4=1; i4<=K; i4++) if(itd3->i==i4)
 { R[i4][j]=itd3->Rij;}
PermLim[j-1]=Multinomial(d,t);
a.erase(a.begin(),a.end());
t.erase(t.begin(),t.end());
```

```
    s.erase(s.begin(),s.end());
  }
}

void Setn()
{
 for(int i=1; i<=K; i++) for(int j=1; j<=b; j++) n[i][j]=0;
 for(int i=0; i<d; i++) for(int j=0; j<b; j++)
 { int k=D[i][j]; n[k][j+1]=1;}
}

void SetSigma() //Cov(R[i1,+],R[i2,+])
{
  double TieFactor;
  for(int i1=1; i1<K; i1++) for(int i2=1; i2<K; i2++)
  {
    Sigma[i1][i2]=0;
    for(int j=1; j<=b; j++)
    {
      TieFactor=(1.0-gammaj[j-1]/((d-1.0)*d*(d+1.0)))/12.0;
      if(i1==i2) { if(n[i1][j]==1)
       Sigma[i1][i1]+=(d-1.0)*(d+1.0)*TieFactor;}
      else { if(n[i1][j]==1 && n[i2][j]==1)
       Sigma[i1][i2]-=(d+1.0)*TieFactor;}
    }
  }
}

void SetCholeski() //Sigma=LL' where L is lower triangular
{
  double lamMin=1.0E25, lamMax=0;
  for(int i1=1; i1<=K-1; i1++)
   for(int i2=1; i2<=i1; i2++)
   {
    sum=0;
    L[i1][i2]=Sigma[i1][i2];
    for(int j1=1; j1<i2; j1++) sum+=L[i1][j1]*L[i2][j1];
    L[i1][i2]-=sum;
```

```
    if(i1==i2)
    {
      lamMin=min(L[i1][i1],lamMin);
      lamMax=max(L[i1][i1],lamMax);
      if(lamMax<epsilon||(lamMin/lamMax)<epsilon)
       {
         cout<<"The covariance matrix Sigma is singular. ";
 cout<<"Program exit.\n";
         exit(0);
       }
      L[i1][i1]=sqrt(L[i1][i1]);
    }
    else L[i1][i2]/=L[i2][i2];
  }
}

void SetU()
{
  for(int i=1; i<=K; i++)
  {
    Ri[i]=0;
    for(int j=1; j<=b; j++) Ri[i]+=R[i][j];
  }
  int a0=0; //number of times each treatment occurs
  for(int i=0; i<d; i++) for(int j=0; j<b; j++)
                          if(D[i][j]==1) a0++;
  double ERi=a0*(d+1.0)/2.0;
  for(int i=1; i<=K; i++) U[i]=Ri[i]-ERi;
}

double DurbanStat() // U=LW, Sigma=LL', Q=W'W
{
  double sum;
  double Q1=0;
  for(int i1=1; i1<K; i1++)
  {
    sum=0;
    for(int k=1; k<i1; k++) sum+=L[i1][k]*W[k];
```

```
    W[i1]=(U[i1]-sum)/L[i1][i1];
    Q1+=sqr(W[i1]);
  }
  return Q1;
}

void ApproxPvalue()
{
  Q=DurbanStat();
  cout<<"Value of Durban statistic is Q="<<Q<<" .\n";
  cout<<"Approximate P-value: P[ChiSquare("<<K-1<<")>"<<Q<<"]=";
  cout<<1.0-cdf::icgamma(Q/2.0,(K-1.0)/2.0)<<" .\n";
}

bool PermuteZ()
{
  int k=0;
  for(k=0; k<(b-1); k++)
   { if(PermCount[k]<(PermLim[k]-1)) break;}
   if(k<(b-1))
    {
     next_permutation(Z[k].begin(),Z[k].end());
     PermCount[k]++;
     for(int i=0; i<k; i++) PermCount[i]=0;
     return true;
    }
   else return false;
}

void ExactPvalue()
{
  const double delta=1.0E-5;
  char ch;
  long PermTotal=1;
  for(int i=0; i<(b-1); i++) PermTotal*=PermLim[i];
  cout<<"For calculating the exact P-value, the total ";
  cout<<"number of permutations is "<<PermTotal<<".\n";
  cout<<"Do you wish to continue? Type Y)es or N)o :"; cin>>ch;
```

```
  if(ch=='N'||ch=='n') exit(0);
  else while(ch!='N'&&ch!='n'&&ch!='Y'&&ch!='y')
   { cout<<"Please type Y,y,N,or n :"; cin>>ch; }
  if(ch=='N'||ch=='n') exit(0);
  double Q0;
  countN=0, countD=0;
  for(int i=0; i<(b-1); i++) PermCount[i]=0;
  do
  {
    SetRMatrix();
    SetU();
    Q0=DurbanStat();
    if(Q0>=(Q-delta)) countN++; countD++;
  }while(PermuteZ());
  cout<<"The exact P-value is: "<<countN;
  cout<<"/"<<countD<<"="<<((double)countN)/((double)countD)<<" .\n";
}

void CleanUp()
{
 for(int i=0; i<d;  i++) delete[]D[i]; delete[]D;
 for(int i=0; i<=K; i++) delete[]R[i]; delete[]R;
 for(int i=0; i<=K; i++) delete L[i];  delete[]L;
 for(int i=0; i<=K; i++) delete n[i];  delete[]n;
 delete[]U; delete[]W; delete[]Ri; delete[]Z;
 delete[]PermLim; delete[]PermCount;
}

int main(int argc, char *argv[])
{
  int count=0;
  Heading();
  GetDMatrix(argv[1]);
  PrintDMatrix();
  SetStorage();
  GetZMatrix(argv[2]);
  PrintZVector();
  SetRMatrix();
```

```
  Setn();
  SetSigma();
  SetCholeski();
  SetU();
  ApproxPvalue();
  ExactPvalue();
  CleanUp();
  return 0;
}
```

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Index