# Evaluation and Credibility

How much should we believe in what was learned?

# Outline

- Introduction
- Classification with Train, Test, and Validation sets
  - Handling Unbalanced Data; Parameter Tuning
- Cross-validation
- Comparing Data Mining Schemes

# Introduction

- How predictive is the model we learned?
- Error on the training data is *not* a good indicator of performance on future data
  - ***Q: Why?***
  - A: Because new data will probably not be **exactly** the same as the training data!
- Overfitting – fitting the training data too precisely - usually leads to poor results on new data

# Evaluation issues

- Possible evaluation measures:
  - Classification Accuracy
  - Total cost/benefit – when different errors involve different costs
  - Lift and ROC curves
  - Error in numeric predictions
- How reliable are the predicted results ?

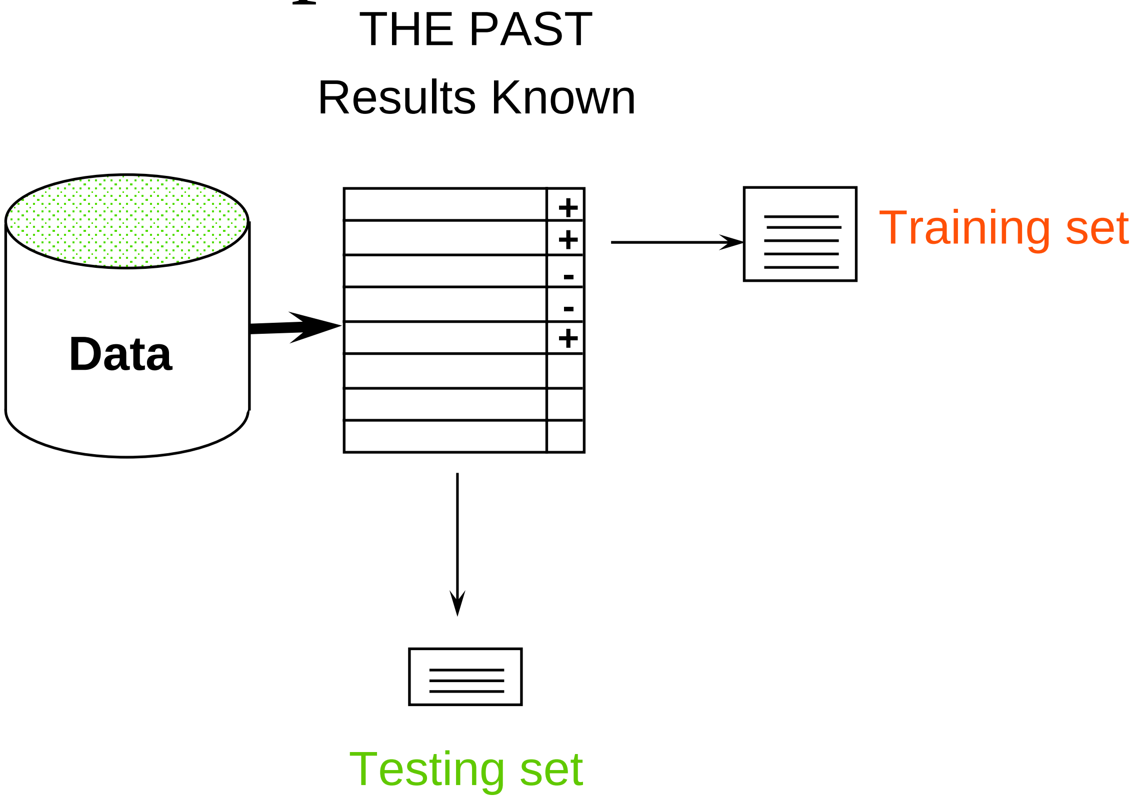
# Classifier error rate

- Natural performance measure for classification problems: *error rate*
  - *Success*: instance's class is predicted correctly
  - *Error*: instance's class is predicted incorrectly
  - Error rate: proportion of errors made over the whole set of instances
- *Training set error rate:* is way too optimistic!
  - you can find patterns even in random data

# Evaluation on “LARGE” data

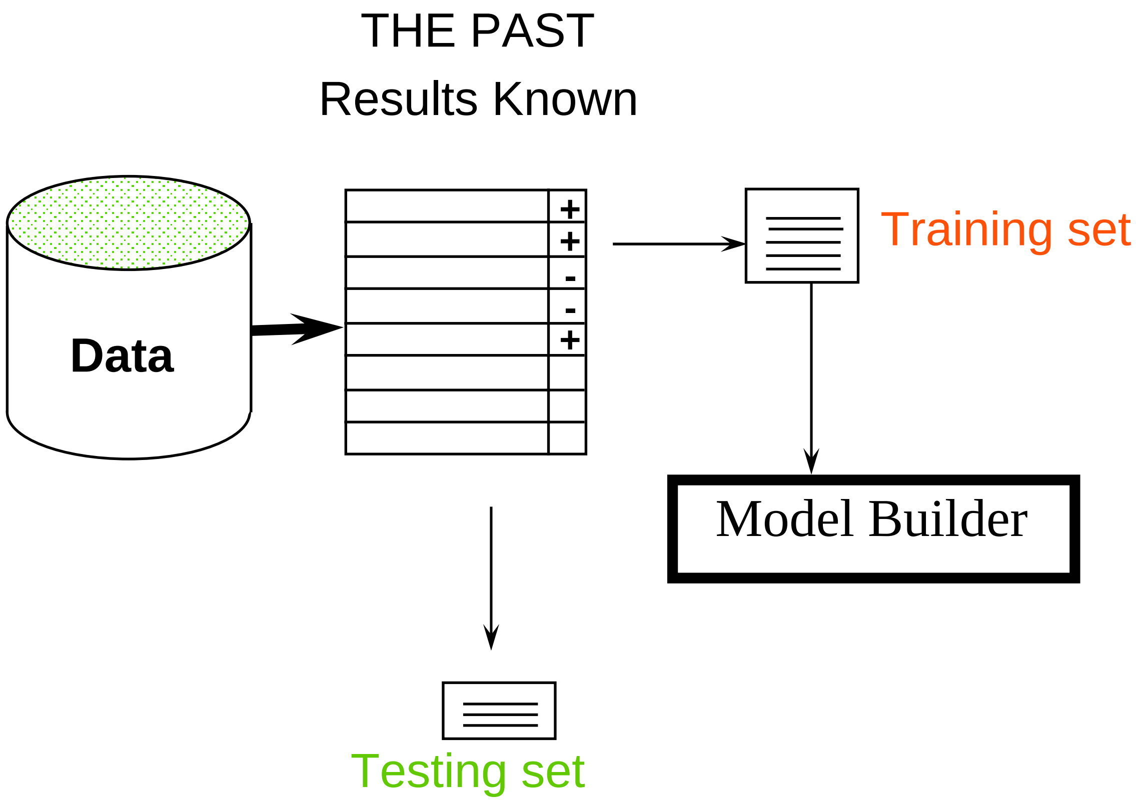
- If many (thousands) of examples are available, including several hundred examples from each class, then a simple evaluation is sufficient
  - Randomly split data into training and test sets (usually 2/3 for train, 1/3 for test)
- Build a classifier using the *train* set and evaluate it using the *test* set.

# Classification Step 1:
# Split data into train and test sets

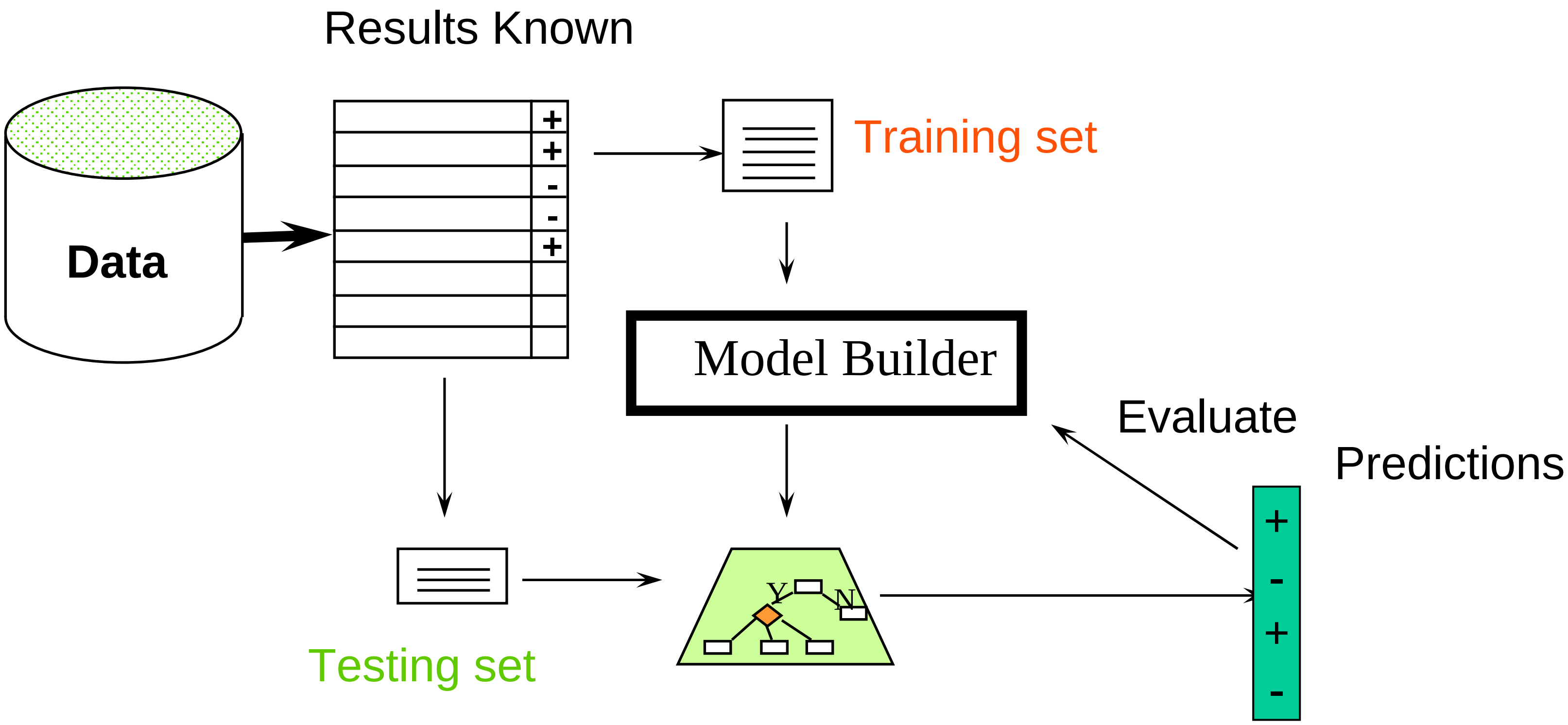


# Classification Step 2:

# Build a model on a training set



# Classification Step 3:
# Evaluate on test set (Re-train?)



# Handling unbalanced data

- Sometimes, classes have very unequal frequency
  - Attrition prediction: 97% stay, 3% attrite (in a month)
  - medical diagnosis: 90% healthy, 10% disease
  - eCommerce: 99% don’t buy, 1% buy
  - Security: >99.99% of Americans are not terrorists
- Similar situation with multiple classes
- Majority class classifier can be 97% correct

# Balancing unbalanced data

- With two classes, a good approach is to build **BALANCED** train and test sets, and train model on a balanced set
  - randomly select desired number of minority class instances
  - add equal number of randomly selected majority class
- Generalize "balancing" to multiple classes
  - Ensure that each class is represented with approximately equal proportions in train and test

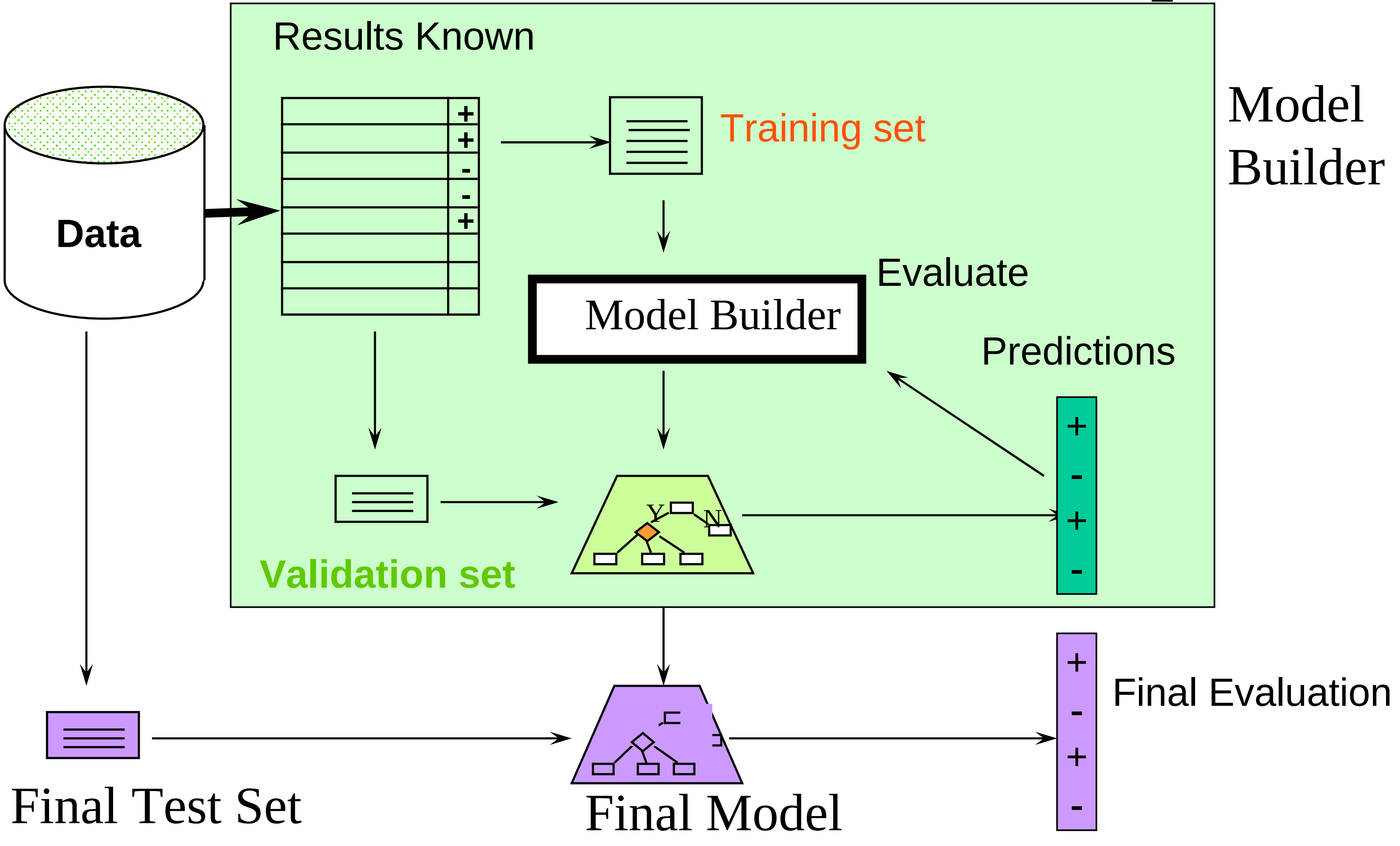
# A note on parameter tuning

- It is important that the test data is not used *in any way* to create the classifier
- Some learning schemes operate in two stages:
  - Stage 1: builds the basic structure
  - Stage 2: optimizes parameter settings
- The test data can’t be used for parameter tuning!
- Proper procedure uses three sets: **training data, validation data, and test data**
  - Validation data is used to optimize parameters

# Making the most of the data

- Once evaluation is complete, *all the data* can be used to build the final classifier
- Generally, the larger the training data the better the classifier (but returns diminish)
- The larger the test data the more accurate the error estimate

# Classification: Train, Validation, Test split



# *Predicting performance

- Assume the estimated error rate is 25%. How close is this to the true error rate?
  - Depends on the amount of test data
- Prediction is just like tossing a biased (!) coin
  - “Head” is a “success”, “tail” is an “error”
- In statistics, a succession of independent events like this is called a Bernoulli process
- Statistical theory provides us with confidence intervals for the true underlying

# *Confidence intervals

- We can say: $p$ lies within a certain specified interval with a certain specified confidence
- Example: $S$=750 successes in $N$=1000 trials
  - Estimated success rate: 75%
  - How close is this to true success rate $p$?
    - Answer: with 80% confidence $p \in [73.2, 76.7]$
- Another example: $S$=75 and $N$=100
  - Estimated success rate: 75%
  - With 80% confidence $p \in [69.1, 80.1]$

# *Mean and variance (also Mod 7)

- Mean and variance for a Bernoulli trial:
  $p$, $p\,(1–p)$
- Expected success rate $f=S/N$
- Mean and variance for $f$ : $p$, $p\,(1–p)/N$
- For large enough $N$, $f$ follows a Normal distribution
- c% confidence interval $[–z \le X \le z]$ for random variable with 0 mean is given by:

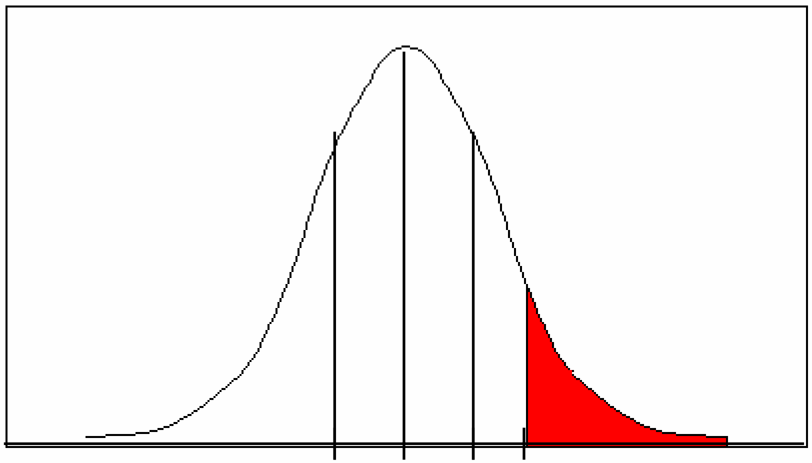
$$\Pr[-z \le X \le z] = c$$

- With a symmetric distribution:

$$\Pr[-z \le X \le z] = 1 - 2 \times \Pr[X \ge z]$$

# *Confidence limits

- Confidence limits for the normal distribution with 0 mean and a variance of 1:




| Pr[$X \geq z$] | $z$ |
|---|---|
| 0.1% | 3.09 |
| 0.5% | 2.58 |
| 1% | 2.33 |
| 5% | 1.65 |
| 10% | 1.28 |
| 20% | 0.84 |
| 40% | 0.25 |

- Thus:

$$\Pr[-1.65 \leq X \leq 1.65] = 90\%$$

- To use this we have to reduce our random variable $f$ to have 0 mean and unit variance

# *Transforming *f*

- Transformed value for *f* : $\dfrac{f-p}{\sqrt{p(1-p)/N}}$

  (i.e. subtract the mean and divide by the *standard deviation*)

- Resulting equation: $\Pr\left[-z \le \dfrac{f-p}{\sqrt{p(1-p)/N}} \le z\right] = c$

- Solving for *p* :

$$p = \left( f + \frac{z^2}{2N} \pm z\sqrt{\frac{f}{N} - \frac{f^2}{N} + \frac{z^2}{4N^2}} \right) \Bigg/ \left(1 + \frac{z^2}{N}\right)$$

# *Examples

- $f$ = 75%, $N$ = 1000, $c$ = 80% (so that $z = 1.28$): $p \in [0.732, 0.767]$
- $f$ = 75%, $N$ = 100, $c$ = 80% (so that $z = 1.28$): $p \in [0.691, 0.801]$
- Note that normal distribution assumption is only valid for large $N$ (i.e. $N$ > 100)
- $f$ = 75%, $N$ = 10, $c$ = 80% (so that $z = 1.28$): $p \in [0.549, 0.881]$

(should be taken with a grain of salt)

# Evaluation on “small” data

- The *holdout* method reserves a certain amount for testing and uses the remainder for training
  - Usually: one third for testing, the rest for training
- For small or “unbalanced” datasets, samples might not be representative
  - Few or none instances of some classes
- *Stratified sample: advanced version of balancing the data*
  - Make sure that each class is represented with approximately equal proportions in both subsets

# Repeated holdout method

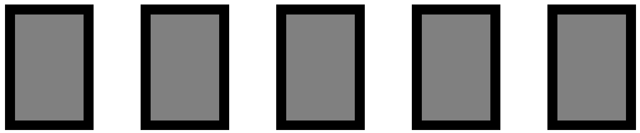
- Holdout estimate can be made more reliable by repeating the process with different subsamples
  - In each iteration, a certain proportion is randomly selected for training (possibly with stratification)
  - The error rates on the different iterations are averaged to yield an overall error rate
- This is called the *repeated holdout* method
- Still not optimum: the different test sets

# Cross-validation

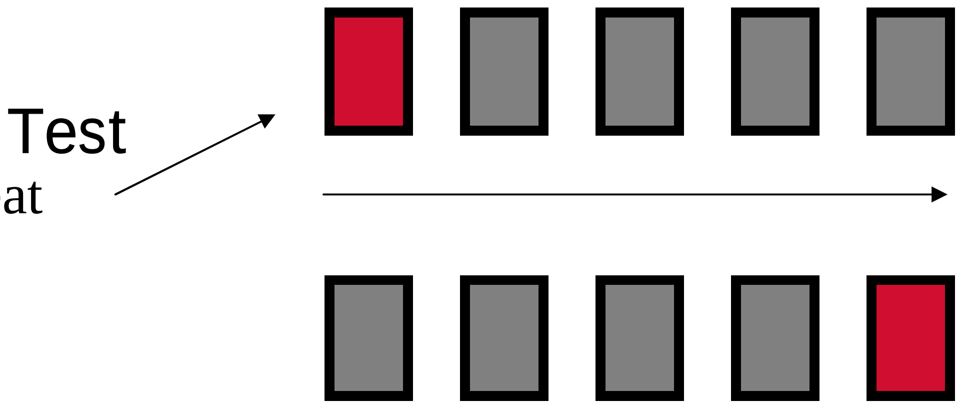
- *Cross-validation* avoids overlapping test sets
  - First step: data is split into *k* subsets of equal size
  - Second step: each subset in turn is used for testing and the remainder for training
- This is called *k-fold cross-validation*
- Often the subsets are stratified before the cross-validation is performed
- The error estimates are averaged to yield an overall error estimate

# Cross-validation example:

- Break up data into groups of the same size



- Hold aside one group for testing and use the rest to build model




- Repeat

# More on cross-validation

- Standard method for evaluation: stratified ten-fold cross-validation
- Why ten? Extensive experiments have shown that this is the best choice to get an accurate estimate
- Stratification reduces the estimate’s variance
- Even better: repeated stratified cross-validation
  - E.g. ten-fold cross-validation is repeated ten

# Leave-One-Out cross-validation

- Leave-One-Out:
  a particular form of cross-validation:
  - Set number of folds to number of training instances
  - I.e., for *n* training instances, build classifier *n* times
- Makes best use of the data
- Involves no random subsampling
- Very computationally expensive
  - (exception: NN)

# Leave-One-Out-CV and stratification

- Disadvantage of Leave-One-Out-CV: stratification is not possible
  - It *guarantees* a non-stratified sample because there is only one instance in the test set!
- Extreme example: random dataset split equally into two classes
  - Best inducer predicts majority class
  - 50% accuracy on fresh data
  - Leave-One-Out-CV estimate is 100% error!

# *The bootstrap

- CV uses sampling *without replacement*
  – The same instance, once selected, can not be selected again for a particular training/test set
- The *bootstrap* uses sampling *with replacement* to form the training set
  – Sample a dataset of *n* instances *n* times *with replacement* to form a new dataset of *n* instances
  – Use this data as the training set
  – Use the instances from the original dataset that don't occur in the new training set for testing

# *The 0.632 bootstrap

- Also called the *0.632 bootstrap*
  - A particular instance has a probability of 1–1/*n* of *not* being picked
  - Thus its probability of ending up in the test data is:

$$\left(1-\frac{1}{n}\right)^{n} \approx e^{-1} = 0.368$$

  - This means the training data will contain approximately 63.2% of the instances

# *Estimating error with the bootstrap

- The error estimate on the test data will be very pessimistic
  - Trained on just ~63% of the instances
- Therefore, combine it with the resubstitution error:

$$err = 0.632 \cdot e_{\text{test instances}} + 0.368 \cdot e_{\text{training instances}}$$

- The resubstitution error gets less weight than the error on the test data
- Repeat process several times with different replacement samples; average the results

# *More on the bootstrap

- Probably the best way of estimating performance for very small datasets
- However, it has some problems
  - Consider the random dataset from above
  - A perfect memorizer will achieve
    0% resubstitution error and
    ~50% error on test data
  - Bootstrap estimate for this classifier:

$$err = 0.632 \cdot 50\% + 0.368 \cdot 0\% = 31.6\%$$

  - True expected error: 50%

# Comparing data mining schemes

- Frequent situation: we want to know which one of two learning schemes performs better
- Note: this is domain dependent!
- Obvious way: compare 10-fold CV estimates
- Problem: variance in estimate
- Variance can be reduced using repeated CV
- However, we still don't know whether the results are reliable

# Direct Marketing Paradigm

- Find most likely prospects to contact
- Not everybody needs to be contacted
- Number of targets is usually much smaller than number of prospects

- Typical Applications
  - retailers, catalogues, direct mail (and e-mail)
  - customer acquisition, cross-sell, attrition prediction
  - ...

# Direct Marketing Evaluation

- **Accuracy on the entire dataset is not the right measure**
- Approach
  - develop a target model
  - score all prospects and rank them by decreasing score
  - select top P% of prospects for action
- How to decide what is the best selection?

# Model-Sorted List

Use a model to assign score to each customer
Sort customers by decreasing score
Expect more targets (hits) near the top of the list

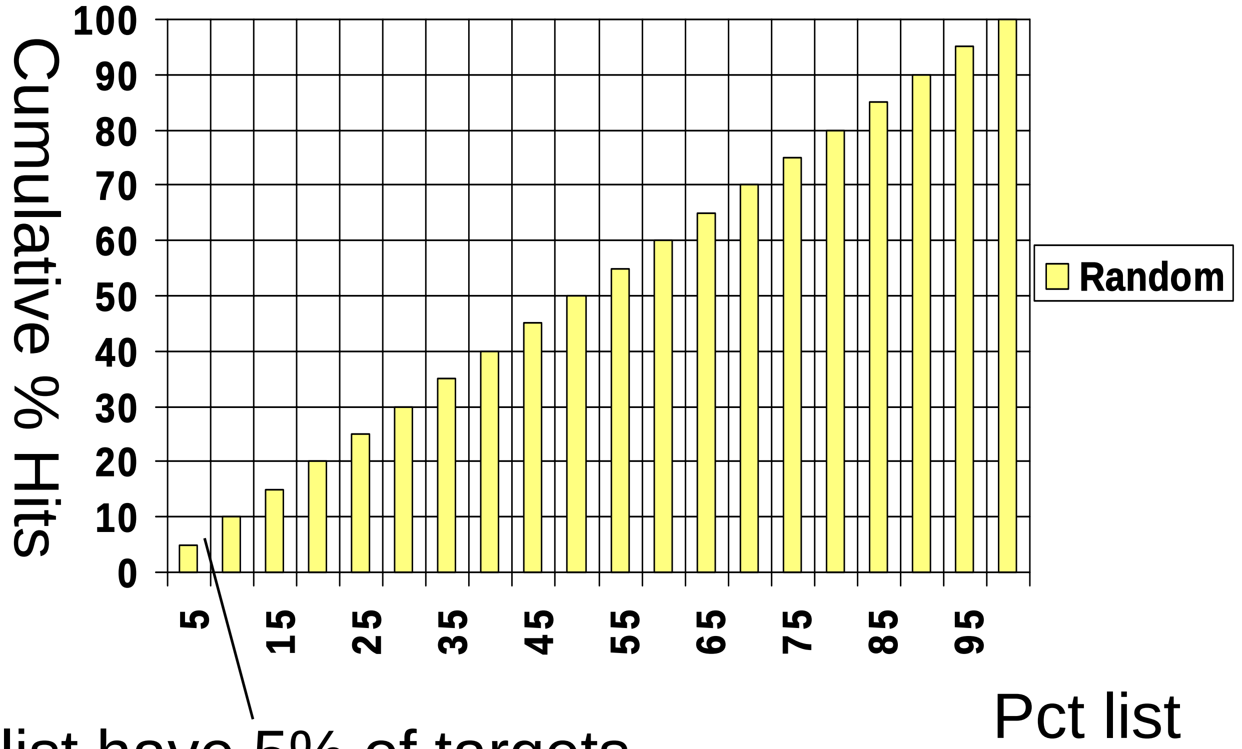
| No | Scor | Targe | CustI | Ag | |
|---|---|---|---|---|---|
| 1 | 0.97 | Y | 1746 | … | |
| 2 | 0.95 | N | 1024 | … | |
| 3 | 0.94 | Y | 2478 | … | |
| 4 | 0.93 | Y | 3820 | … | |
| 5 | 0.92 | N | 4897 | … | |
| … | … | | … | … | |
| 99 | 0.11 | N | 2734 | … | |
| 100 | 0.06 | N | 2422 | | |

3 hits in top 5% of the list

If there 15 targets overall, then top 5 has 3/15=20% of targets

# CPH (Cumulative Pct Hits)

**Definition:**
**CPH(P,M)**
**= % of all targets in the first P% of the list scored by model M**
**CPH frequently called Gains**

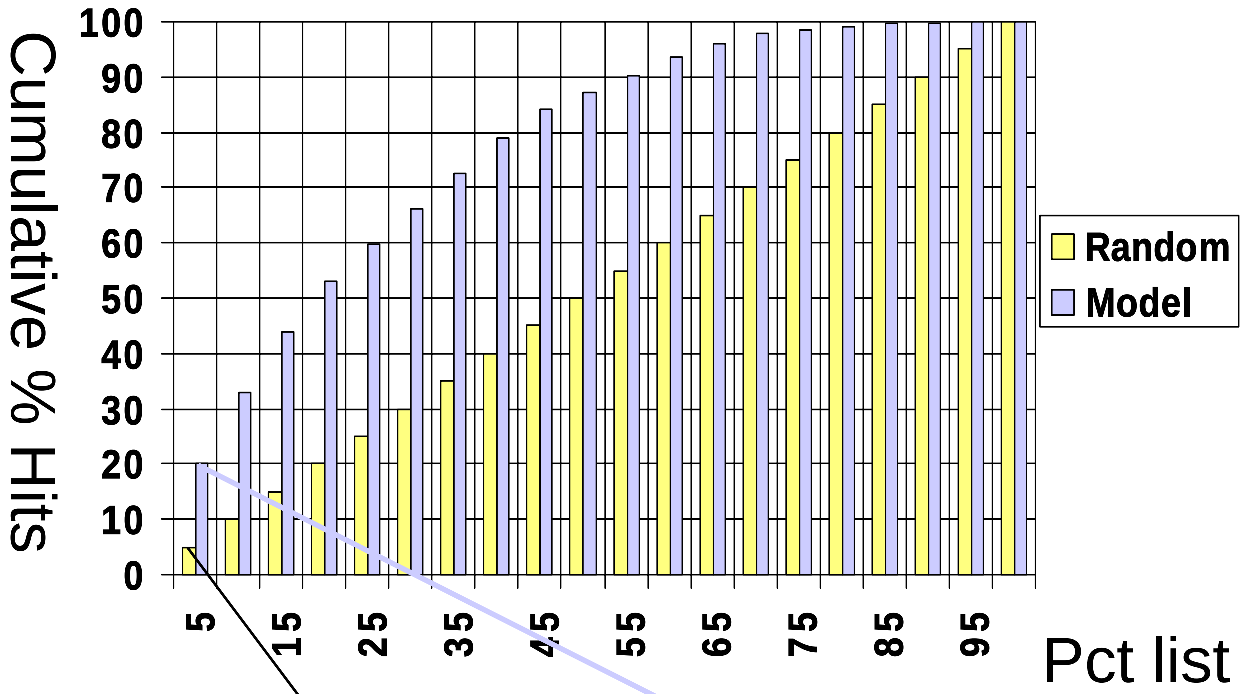



5% of random list have 5% of targets

*Q: What is expected value for CPH(P,Random) ?*

**A: Expected value for CPH(P,Random) = P**

# CPH: Random List vs Model-ranked list




5% of random list have 5% of targets,

but 5% of model ranked list have 21% of targets
CPH(5%,model)=21%.

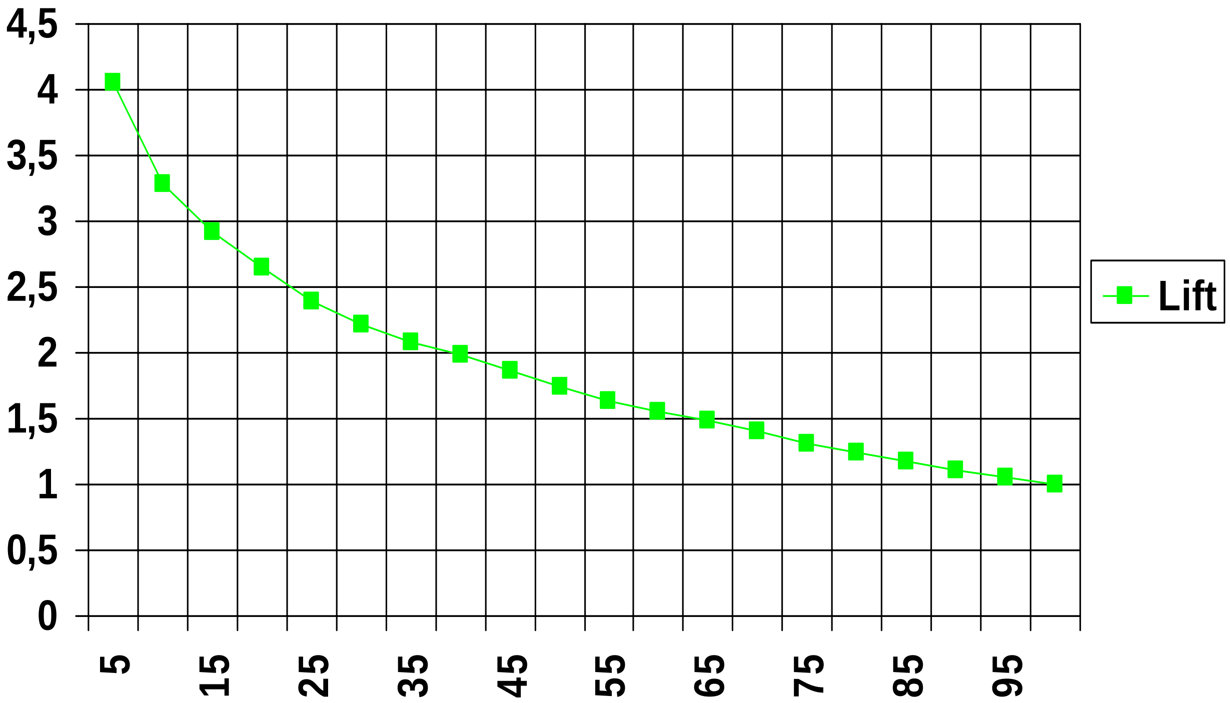
# Lift

$$\mathbf{Lift}(P,M) = \mathbf{CPH}(P,M) \;/\; P$$

Lift (at 5%)

= 21% / 5%

= 4.2 better than random




P -- percent of the list

*Note: Some (including Witten & Eibe) use "Lift" for what we call CPH.*

# Lift Properties

- ***Q: Lift(P,Random) =***
  - ***A:*** 1 (expected value, can vary)
- ***Q: Lift(100%, M) =***
  - ***A:*** 1 (for any model M)
- ***Q: Can lift be less than 1?***
  - ***A***: yes, if the model is inverted (all the non-targets precede targets in the list)
- Generally, a better model has higher lift

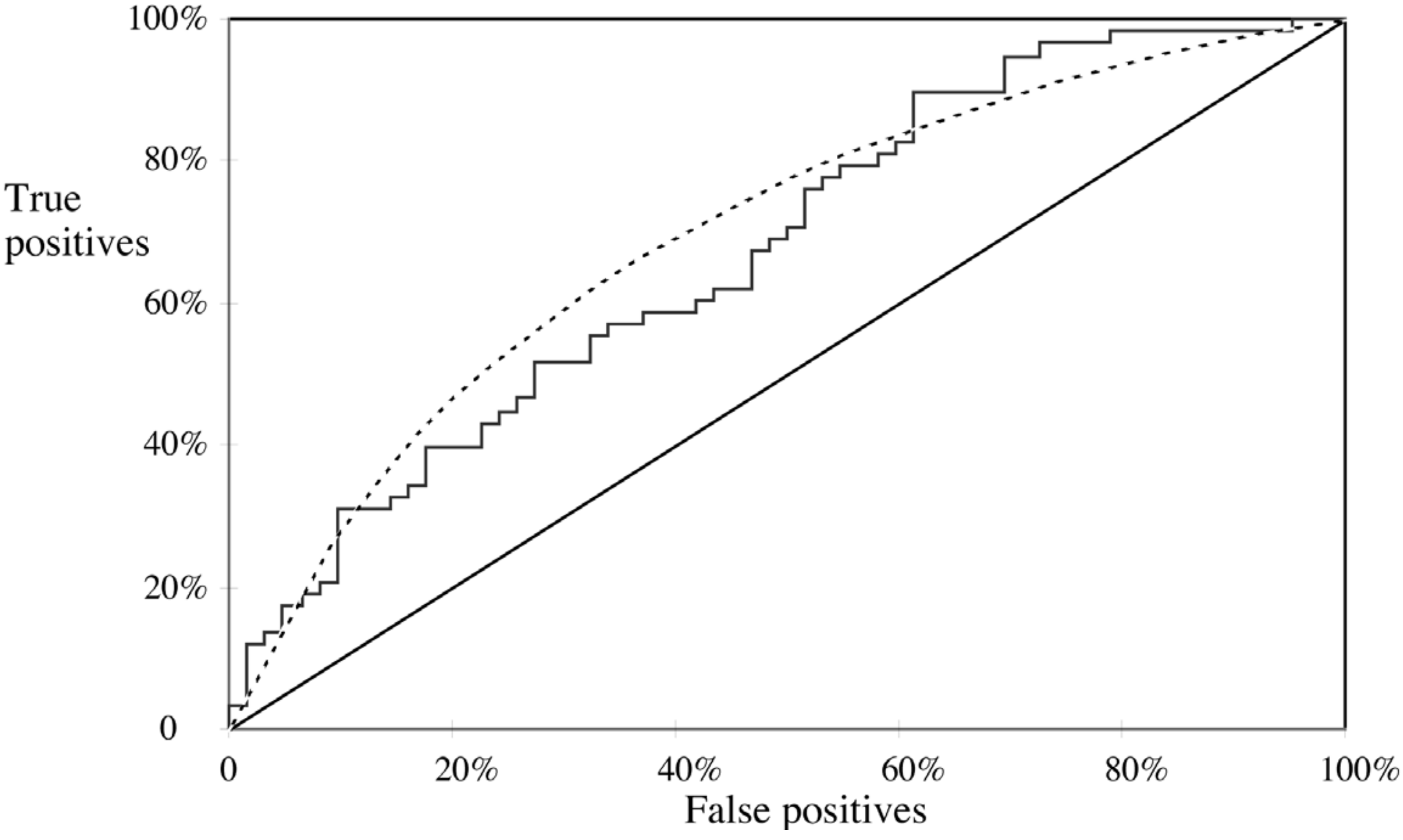
# *ROC curves

- *ROC curves* are similar to gains charts
  - Stands for “receiver operating characteristic”
  - Used in signal detection to show tradeoff between hit rate and false alarm rate over noisy channel
- Differences from gains chart:
  - *y* axis shows percentage of true positives in sample

    *rather than absolute number*
  - *x* axis shows percentage of false positives in sample

    *rather than sample size*

# *A sample ROC curve



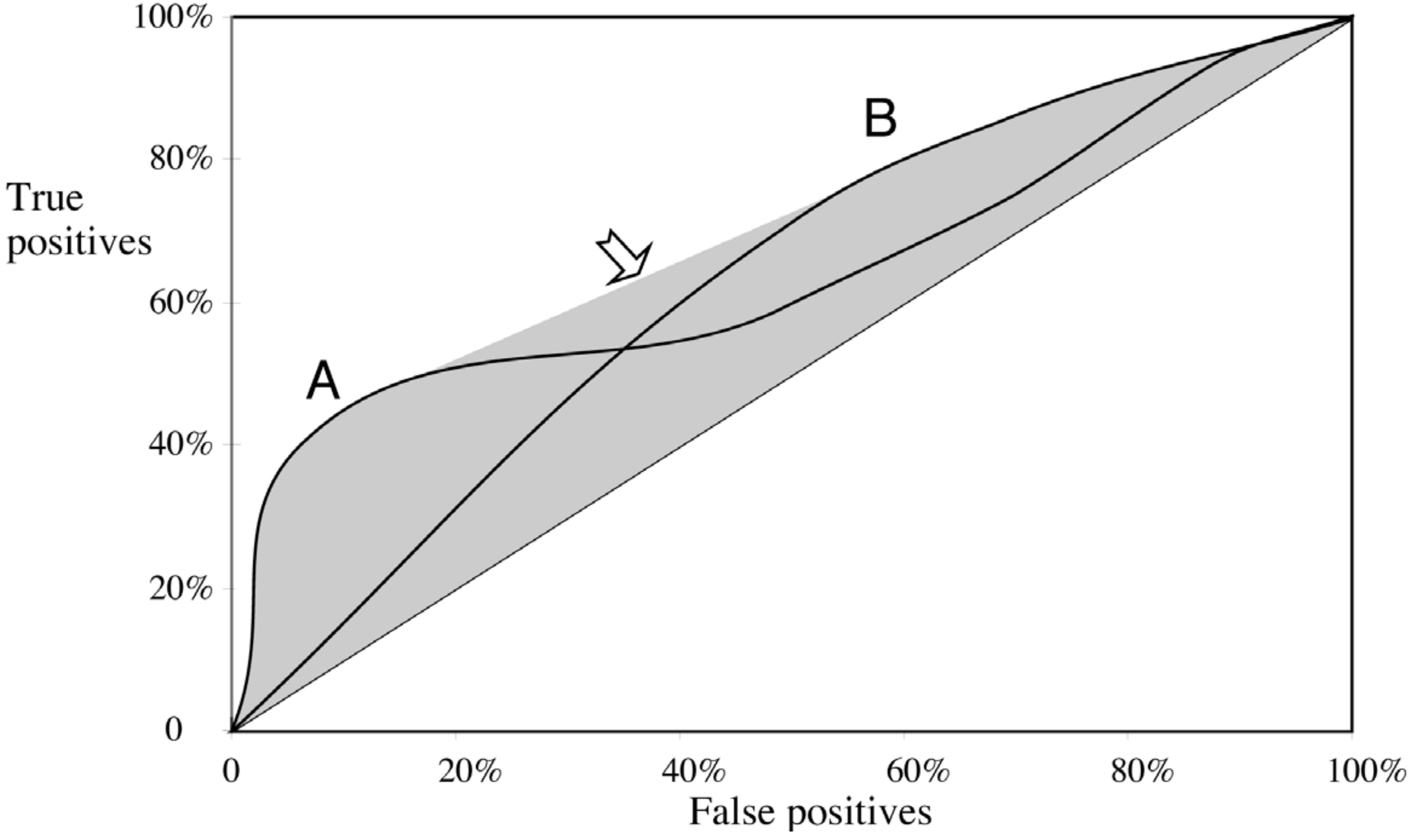

- Jagged curve—one set of test data
- Smooth curve—use cross-validation

witten & eibe

# *Cross-validation and ROC curves

- Simple method of getting a ROC curve using cross-validation:
  - Collect probabilities for instances in test folds
  - Sort instances according to probabilities
- This method is implemented in WEKA
- However, this is just one possibility
  - The method described in the book generates an ROC curve for each fold and averages them

# *ROC curves for two schemes




- For a small, focused sample, use method A
- For a larger one, use method B
- In between, choose between A and B with appropriate probabilities

# *The convex hull

- Given two learning schemes we can achieve any point on the convex hull!
- TP and FP rates for scheme 1: $t_1$ and $f_1$
- TP and FP rates for scheme 2: $t_2$ and $f_2$
- If scheme 1 is used to predict $100 \times q$ % of the cases and scheme 2 for the rest, then
  - TP rate for combined scheme:
    $q \times t_1 + (1-q) \times t_2$
  - FP rate for combined scheme:
    $q \times f_2 + (1-q) \times f_2$

# Cost Sensitive Learning

- There are two types of errors

| | | Predicted class | |
|---|---|---|---|
| | | Yes | No |
| **Actual class** | Yes | TP: True positive | FN: False negative |
| | No | FP: False positive | TN: True negative |

- Machine Learning methods usually minimize FP+FN
- Direct marketing maximizes TP

# Different Costs

- In practice, true positive and false negative errors often incur different costs
- Examples:
  - Medical diagnostic tests: does X have leukemia?
  - Loan decisions: approve mortgage for X?
  - Web mining: will X click on this link?
  - Promotional mailing: will X buy the product?
  - …

# Cost-sensitive learning

- Most learning schemes do not perform cost-sensitive learning
  - They generate the same classifier no matter what costs are assigned to the different classes
  - Example: standard decision tree learner
- Simple methods for cost-sensitive learning:
  - Re-sampling of instances according to costs
  - Weighting of instances according to costs
- Some schemes are inherently cost-sensitive, e.g. naïve Bayes

# KDD Cup 98 – a Case Study

- Cost-sensitive learning/data mining widely used, but rarely published
- Well known and public case study: KDD Cup 1998
  - Data from Paralyzed Veterans of America (charity)
  - Goal: select mailing with the highest profit
  - Evaluation: Maximum actual profit from selected list (with mailing cost = $0.68)
    - Sum of (actual donation-$0.68) for all records with predicted/ expected donation > $0.68
- More in a later lesson

# *Measures in information retrieval

- Percentage of retrieved documents that are relevant: *precision*=TP/(TP+FP)
- Percentage of relevant documents that are returned: *recall* =TP/(TP+FN)
- Precision/recall curves have hyperbolic shape
- Summary measures: average precision at 20%, 50% and 80% recall (*three-point average recall*)
- *F-measure*=(2×recall×precision)/(recall+precision)

# *Summary of measures

| | Domain | Plot | Explanation |
|---|---|---|---|
| **Lift chart** | **Marketing** | **TP**<br>**Subset size** | **TP**<br>**(TP+FP)/(TP+FP+TN+FN)** |
| **ROC curve** | **Communications** | **TP rate**<br>**FP rate** | **TP/(TP+FN)**<br>**FP/(FP+TN)** |
| **Recall-precision curve** | **Information retrieval** | **Recall**<br>**Precision** | **TP/(TP+FN)**<br>**TP/(TP+FP)** |