

Linear Algebra

Lecture 14 - Quadratic Forms

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Quadratic Form

Definition

A function $Q: \mathbb{R}^n \longrightarrow \mathbb{R}$ is called a **quadratic form** if

$$Q((x_1, \dots, x_n)) = a_{11}x_1^2 + \dots + a_{nn}x_n^2 + \sum_{1 \leq i < j \leq n} a_{ij}x_i x_j,$$

that is, it is a function given by a homogeneous polynomial of degree 2 in variables x_1, \dots, x_n .

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$$Q((x_1, x_2)) = x_1^2 - x_2^2$$

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Examples

$$Q((x_1, x_2)) = x_1^2 - x_2^2$$

$$Q((x_1, x_2, x_3)) = x_1^2 + 2x_2^2 + 5x_3^2 + 2x_1x_2 - 2x_1x_3 + 2x_2x_3$$

Symmetric Matrix

Recall

Definition

Matrix $A = [a_{ij}] \in M(n \times n; \mathbb{R})$ is called **symmetric** if $A^T = A$, i.e. $a_{ij} = a_{ji}$ for $i, j = 1, \dots, n$.

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matrix $\begin{bmatrix} 0 & 2 & 5 \\ 2 & 4 & -3 \\ 5 & -3 & 1 \end{bmatrix}$ is symmetric

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matrix $\begin{bmatrix} 0 & 2 & 5 \\ 2 & 4 & -3 \\ 5 & -3 & 1 \end{bmatrix}$ is symmetric

matrix $\begin{bmatrix} 0 & 2 & 6 \\ 2 & 4 & -3 \\ 5 & -3 & 1 \end{bmatrix}$ is not symmetric

Matrix of a Quadratic Form

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Let $Q((x_1, \dots, x_n)) = \sum_{i=1}^n a_{ii}x_i^2 + \sum_{1 \leq i < j \leq n} a_{ij}x_i x_j$ be a quadratic form. The matrix of the quadratic form Q is a symmetric matrix $M = [b_{ij}] \in M(n \times n; \mathbb{R})$ such that $b_{ii} = a_{ii}$ and $b_{ij} = b_{ji} = \frac{1}{2}a_{ij}$ for $1 \leq i < j \leq n$.

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The matrix of the form $Q((x_1, x_2)) = x_1^2 - x_2^2$ is $M = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$.

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The matrix of the form $Q((x_1, x_2, x_3)) = x_1^2 + 2x_2^2 + 5x_3^2 + 2x_1x_2 - 4x_1x_3 + 8x_2x_3$ is

$$M = \begin{bmatrix} 1 & 1 & -2 \\ 1 & 2 & 4 \\ -2 & 4 & 5 \end{bmatrix}$$

Matrix of a Quadratic Form (continued)

Proposition

Let M be a matrix of the quadratic form $Q: \mathbb{R}^n \longrightarrow \mathbb{R}$. Then

$$Q((x_1, \dots, x_n)) = x^T M x,$$

where $x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}.$

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Proof.

Entries of matrix M in the i -th row get multiplied by x_i and elements in the j -th column get multiplied by x_j . For every $i \neq j$ the monomial $x_i x_j$ comes from the entry in the i -th row, j -th column and from the entry in the j -th row, i -th column. □

Matrix of a Quadratic Form (continued)

Formal explanation

$$\begin{aligned} Q((x_1, \dots, x_n)) &= x^T M x = \begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \begin{bmatrix} \sum_{s=1}^n b_{1s} x_s \\ \sum_{s=1}^n b_{2s} x_s \\ \vdots \\ \sum_{s=1}^n b_{ns} x_s \end{bmatrix} = \\ &= x_1 \sum_{s=1}^n b_{1s} x_s + x_2 \sum_{s=1}^n b_{2s} x_s + \dots + x_n \sum_{s=1}^n b_{ns} x_s = \\ &= \sum_{i,j=1}^n b_{ij} x_i x_j. \end{aligned}$$

Positive/Negative Definite Quadratic Form

Definition

Quadratic form $Q: \mathbb{R}^n \longrightarrow \mathbb{R}$ (resp. symmetric matrix $M \in M(n \times n; \mathbb{R})$) is **positive definite** if $Q(x) > 0$ (resp. $x^T M x > 0$) for any $x \in \mathbb{R}^n$, $x \neq \mathbf{0}$.

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The quadratic form $\|\cdot\|^2: \mathbb{R}^n \longrightarrow \mathbb{R}$ is positive definite since $\|x\|^2 = x_1^2 + \dots + x_n^2 > 0$ for $x \neq \mathbf{0}$.

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The quadratic form $Q((x_1, x_2, x_3)) = x_1^2 + 2x_2^2 + 5x_3^2 + 2x_1x_2 - 2x_1x_3 + 2x_2x_3 = (x_1 + x_2 - x_3)^2 + (x_2 + 2x_3)^2$ is not positive definite since $Q((3, -2, 1)) = 0$. It is not negative definite.

Recall

$$(a_1 + a_2 + \dots + a_n)^2 = a_1^2 + a_2^2 + \dots + a_n^2 + 2a_1a_2 + 2a_1a_3 + \dots + 2a_1a_n + \\ + 2a_2a_3 + 2a_2a_4 + \dots + 2a_2a_n + 2a_3a_4 + \dots + 2a_3a_n + \dots + 2a_{n-1}a_n$$

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For example

$$(x_1 - 3x_2 + 2x_3)^2 =$$

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For example

$$\begin{aligned}(x_1 - 3x_2 + 2x_3)^2 &= \\&= x_1^2 + (-3)^2x_2^2 + 2^2x_3^2 + 2 \cdot (-3)x_1x_2 + 2 \cdot 2x_1x_3 + 2 \cdot (-3) \cdot 2x_2x_3 = \\&= x_1^2 + 9x_2^2 + 4x_3^2 - 6x_1x_2 + 4x_1x_3 - 12x_2x_3\end{aligned}$$

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Proposition

A quadratic form $Q: \mathbb{R}^n \longrightarrow \mathbb{R}$ can be expressed (possibly after a change of coordinates) as $Q((x_1, \dots, x_n)) = \pm l_1^2 \pm l_2^2 \pm \dots \pm l_n^2$ where l_1, \dots, l_n are linear functions such that l_i, \dots, l_n do not depend on the variables x_1, \dots, x_{i-1} for $i = 2, \dots, n$.

Recall

$$(a_1 + a_2 + \dots + a_n)^2 = a_1^2 + a_2^2 + \dots + a_n^2 + 2a_1a_2 + 2a_1a_3 + \dots + 2a_1a_n + 2a_2a_3 + 2a_2a_4 + \dots + 2a_2a_n + 2a_3a_4 + \dots + 2a_3a_n + \dots + 2a_{n-1}a_n$$

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Proof.

(sketch) Use the above formula.

Example

$$\begin{aligned} Q((x_1, x_2, x_3)) &= x_1^2 + 2x_2^2 + 5x_3^2 + 2x_1x_2 - 2x_1x_3 + 2x_2x_3 = \\ &= (x_1 + x_2 - x_3)^2 + x_2^2 + 4x_2x_3 + 4x_3^2 = (x_1 + x_2 - x_3)^2 + (x_2 + 2x_3)^2 \end{aligned}$$

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Example

$$Q((x_1, x_2, x_3)) = x_1^2 + 2x_2^2 + 5x_3^2 + 2x_1x_2 - 2x_1x_3 + 2x_2x_3 = \\ (x_1 + x_2 - x_3)^2 + x_2^2 + 4x_2x_3 + 4x_3^2 = (x_1 + x_2 - x_3)^2 + (x_2 + 2x_3)^2$$

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What to do if there is no square? Do the following substitution:

$$Q((x_1, x_2, x_3)) = x_1x_2 + 2x_1x_3 = \left\{ \begin{array}{l} x_1 = y_1 - y_2 \\ x_2 = y_1 + y_2 \\ x_3 = y_3 \end{array} \right\} = \\ (y_1 - y_2)(y_1 + y_2) + 2(y_1 - y_2)y_3 = y_1^2 - y_2^2 + 2y_1y_3 - 2y_2y_3 = \\ (y_1 + y_3)^2 - y_2^2 - y_3^2 - 2y_2y_3 = (y_1 + y_3)^2 - (y_2 + y_3)^2$$

Example (continued)

$$Q((x_1, x_2, x_3)) = x_1^2 + 2x_2^2 + 5x_3^2 + 2x_1x_2 - 2x_1x_3 + 2x_2x_3 = \\ (x_1 + x_2 - x_3)^2 + x_2^2 + 4x_2x_3 + 4x_3^2 = (x_1 + x_2 - x_3)^2 + (x_2 + 2x_3)^2$$

Let

$$\begin{cases} y_1 &= x_1 + x_2 - x_3 \\ y_2 &= x_2 + 2x_3 \\ y_3 &= x_3 \end{cases},$$

then $Q((y_1, y_2, y_3)) = y_1^2 + y_2^2$, where

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} = P \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}, \quad \text{for } P = \begin{bmatrix} 1 & 1 & -1 \\ 0 & 1 & 2 \\ 0 & 0 & 1 \end{bmatrix}.$$

In particular

$$y^T \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} y = (P_X)^T \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} P_X = x^T \begin{bmatrix} 1 & 1 & -1 \\ 1 & 2 & 1 \\ -1 & 1 & 5 \end{bmatrix} x.$$

Sylvester's Criterion

Proposition

Let $M \in M(n \times n; \mathbb{R})$ be a symmetric matrix. Let W_i denote the determinant of the upper-left i -by- i submatrix of M . Matrix M is positive definite if and only if $W_i > 0$ for $i = 1, \dots, n$.

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Proof.

Omitted. □

Remark

*The determinants W_i are sometimes called **leading principal minors**.*

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By Sylvester's criterion the quadratic form $x_1^2 + 2x_2^2 + 6x_3^2 + 2x_1x_2 - 2x_1x_3 + 2x_2x_3$ is positive definite.

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A quadratic form Q is positive definite if and only if $-Q$ is negative definite.

Proposition

Let $M \in M(n \times n; \mathbb{R})$ be a symmetric matrix. Let W_i denote the determinant of the upper-left i -by- i submatrix of M . Matrix M is negative definite if and only if

$$W_i < 0 \text{ for odd } i,$$

$$W_i > 0 \text{ for even } i,$$

for $i = 1, \dots, n$.

Example

Consider the symmetric matrix

$$M = \begin{bmatrix} -1 & -1 \\ -1 & -2 \end{bmatrix}$$

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The quadratic form $-x_1^2 - 2x_1x_2 - 2x_2^2 = -(x_1 + x_2)^2 - x_2^2$ is negative definite.

Sylvester's Criterion – Warning

It crucial that matrix A is **symmetric**. For example, let

$$M = \begin{bmatrix} -1 & -3 \\ 1 & 2 \end{bmatrix}.$$

Then

$$\varepsilon_1^T M \varepsilon_1 = -1, \quad \varepsilon_2^T M \varepsilon_2 = 2,$$

hence matrix M is indefinite, however

$$W_1 = -1, \quad W_2 = 1.$$

Postive/Negative Semidefinite Form

Definition

Quadratic form $Q: \mathbb{R}^n \longrightarrow \mathbb{R}$ (resp. symmetric matrix $M \in M(n \times n; \mathbb{R})$) is **positive semidefinite** if $Q(x) \geq 0$ (resp. $x^T M x \geq 0$) for any $x \in \mathbb{R}^n$.

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Quadratic form Q (resp. symmetric matrix M) is **indefinite** if there exist $x, y \in \mathbb{R}^n$ such that $Q(x) > 0, Q(y) < 0$ (resp. $x^T M x > 0, y^T M y < 0$).

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Remark

A positive (resp. negative) definite quadratic form is positive (resp. negative) semidefinite.

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A positive (resp. negative) definite quadratic form is positive (resp. negative) semidefinite. A quadratic form is indefinite if and only if it is not positive semidefinite and it is not negative semidefinite.

Examples

The quadratic form $Q((x_1, x_2)) = x_1^2 - x_2^2$ is indefinite since $Q((1, 0)) > 0$ and $Q((0, 1)) < 0$.

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The quadratic form $Q((x_1, x_2, x_3)) = -x_1^2 - 2x_1x_2 - 2x_2^2 = -(x_1 + x_2)^2 - x_2^2$ is not negative definite since $Q((0, 0, 1)) = 0$. It is negative semidefinite.

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This shows **there is no** direct analogue of Sylvester's criterion for positive/negative semidefinite matrices.

Warning (continued)

Proposition

Let $M \in M(n \times n; \mathbb{R})$ be a symmetric square matrix. Then matrix M is positive semidefinite if and only if for any $J \subset \{1, \dots, n\}, J \neq \emptyset$

$$\det M_{J;J} \geq 0,$$

*that is **all** principal minors are non-negative.*

Warning (continued)

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Proof.

The proof uses spectral theorem and eigenvalue criterion.

(\implies) The restriction of M to the subspace $\text{lin}(\{\varepsilon_i \mid i \in J\})$ is positive semidefinite and has matrix equal to $M_{J;J}$. Since $M_{J;J}$ is symmetric and positive semidefinite, by the eigenvalue criterion $\det M_{J;J}$ is equal to the product of eigenvalues hence it is non-negative.

Warning (continued)

Proof.

(\Leftarrow) Proof by induction on n . Let $Q(x) = x^T M x$ and let $u_1, \dots, u_n \in \mathbb{R}^n$ be an orthonormal basis such that $u_i^T M u_j = 0$ for $i \neq j$. Moreover assume, by rearranging u_i 's, that $Q(u_1) \leq Q(u_2) \leq \dots \leq Q(u_n)$. It is enough to prove $Q(u_1) \geq 0$. If $u_1 \cdot \varepsilon_k = 0$ (i.e. the k -th component of u_1 vanishes) for some $k \in \{1, \dots, n\}$ then $u_1 \in \text{lin}(\varepsilon_1, \dots, \varepsilon_{k-1}, \varepsilon_{k+1}, \dots, \varepsilon_n)$ and $Q(u_1) \geq 0$, by the inductive assumption. Assume $u_1 \cdot \varepsilon_k \neq 0$ for any $k = 1, \dots, n$.

Warning (continued)

Proof.

For $i \geq 2$ and some $k = 1, \dots, n$ consider vector

$$v = (u_i \cdot \varepsilon_k)u_1 - (u_1 \cdot \varepsilon_k)u_i.$$

Since $v \cdot \varepsilon_k = 0$ by the inductive assumption

$$Q(v) = (u_i \cdot \varepsilon_k)^2 Q(u_1) + (u_1 \cdot \varepsilon_k)^2 Q(u_i) \geq 0.$$

If some $Q(u_i) = 0$ with k such that $u_i \cdot \varepsilon_k \neq 0$ (u_i needs to have a non-zero coordinate) then $Q(u_1) \geq 0$. Assume now $Q(u_2), \dots, Q(u_n) > 0$. Then, by choosing $J = \{1, \dots, n\}$ and using the eigenvalue criterion

$$Q(u_1)Q(u_2) \cdot \dots \cdot Q(u_n) \geq 0,$$

that is $Q(u_1) \geq 0$.



Warning (continued)

Remark

Note that for a $n \times n$ matrix there are $2^n - 1$ conditions to check, making this criterion impractical.

Warning (continued)

Corollary

Let $A \in M(n \times n; \mathbb{R})$ be a symmetric square matrix. Then matrix A is negative semidefinite if and only if for any $J \subset \{1, \dots, n\}$, $J \neq \emptyset$

$$\det A_{J;J} \geq 0, \quad \text{when } \#J \text{ is even,}$$

$$\det A_{J;J} \leq 0, \quad \text{when } \#J \text{ is odd,}$$

that is principal minors of M of even order are non-negative and principal minors of M of odd order are non-positive.

Proof.

Matrix M is positive semidefinite if and only if matrix $-M$ is negative semidefinite. □

Warning (continued)

In particular, for

$$M = \begin{bmatrix} 0 & 0 \\ 0 & -1 \end{bmatrix}$$

we have

$$\det M_{1;1} = \det [0] = 0, \quad \det M_{2;2} = \det [-1] = -1 < 0,$$

$$\det M_{1,2;1,2} = \det M = 0,$$

therefore matrix M is not positive semidefinite. In fact, it is negative semidefinite.

Positive Definite Quadratic Form

Proposition

Let $A \in M(m \times n; \mathbb{R})$ be a matrix. Then matrix $M = A^T A \in M(n \times n; \mathbb{R})$ is symmetric and positive semidefinite. Moreover, the matrix $A^T A$ is positive definite if and only if $r(A) = n$ (i.e. columns of matrix A are linearly independent).

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Proof.

For any $x \in \mathbb{R}^n$

$$x^T (A^T A) x = (Ax)^T (Ax) = \|Ax\|^2 \geq 0.$$

(\Leftarrow) If $r(A) = n$ (i.e. the linear transformation $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^m$ given by $A = M(\varphi)_{st}^{st}$ is injective by the rank-nullity theorem) then

$$\|Ax\| = 0 \iff Ax = \mathbf{0} \iff x = \mathbf{0}.$$

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(\Rightarrow) if $Ax = \mathbf{0} \Rightarrow x = \mathbf{0}$ then $\ker \varphi = \{\mathbf{0}\}$ which, by the rank-nullity theorem, gives $r(A) = n$.



Example

Let $A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 1 & 3 \end{bmatrix} \in M(3 \times 2; \mathbb{R})$ where $r(A) = 2$. The matrix

$$A^T A = \begin{bmatrix} 1 & 2 & 1 \\ 2 & 1 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 1 & 3 \end{bmatrix} = \begin{bmatrix} 6 & 7 \\ 7 & 14 \end{bmatrix},$$

is positive definite and the matrix

$$(A^T)^T A^T = A A^T = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 1 & 3 \end{bmatrix} = \begin{bmatrix} 5 & 4 & 7 \\ 4 & 5 & 5 \\ 7 & 5 & 10 \end{bmatrix},$$

is positive semidefinite and it is not positive definite (this will be justified later).

Eigenvalues and Positivity

Theorem (Spectral Theorem)

Symmetric matrix $M \in M(n \times n; \mathbb{R})$ is diagonalizable by an orthonormal eigenbasis.

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In particular, the characteristic polynomial $w_M(\lambda) = \det(M - \lambda I)$ has n real roots (=eigenvalues) counted with multiplicities .

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Theorem

Let $Q: \mathbb{R}^n \longrightarrow \mathbb{R}$ be a quadratic form and let M be its matrix. Let $\lambda_1, \dots, \lambda_n \in \mathbb{R}$ be the roots of $w_M(\lambda)$. Then

- i) form Q is positive definite $\iff \lambda_1, \dots, \lambda_n > 0$,*
- ii) form Q is positive semidefinite $\iff \lambda_1, \dots, \lambda_n \geq 0$,*
- iii) form Q is negative definite $\iff \lambda_1, \dots, \lambda_n < 0$,*
- iv) form Q is negative semidefinite $\iff \lambda_1, \dots, \lambda_n \leq 0$,*
- v) form Q is indefinite $\iff \lambda_i < 0, \lambda_j > 0$ for some $1 \leq i, j \leq n$.*

Eigenvalues and Positivity (continued)

Proof.

Let $v_1, \dots, v_n \in \mathbb{R}^n$ be a basis of \mathbb{R}^n consisting of eigenvectors of M , that is

$$Mv_i = \lambda_i v_i \text{ for } i = 1, \dots, n,$$

where $\lambda_i \in \mathbb{R}$ is an eigenvalue of M and $v_i = \begin{bmatrix} * \\ \vdots \\ * \end{bmatrix} \in M(n \times 1; \mathbb{R})$ is taken to be a n -by-1 matrix.

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$$v_i^T M v_j = v_i^T (M v_j) = v_i^T (\lambda_j v_j) = \lambda_j (v_i \cdot v_j),$$

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$$\begin{aligned} v_i^T M v_j &= v_i^T (M v_j) = v_i^T (\lambda_j v_j) = \lambda_j (v_i \cdot v_j), \\ v_i^T M v_j &= (v_i^T M^T) v_j = (M v_i)^T v_j = (\lambda_i v_i)^T v_j = \lambda_i (v_i \cdot v_j). \end{aligned}$$

This is possible only if $v_i \cdot v_j = 0$, i.e. vectors v_i, v_j are perpendicular.

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Let $v_1, \dots, v_n \in \mathbb{R}^n$ be a basis of \mathbb{R}^n consisting of eigenvectors of M , that is

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This is possible only if $v_i \cdot v_j = 0$, i.e. vectors v_i, v_j are perpendicular. Using Gram-Schmidt process for eigenspaces $V_{(\lambda_i)}$ one can assume the basis v_1, \dots, v_n is orthonormal.

Eigenvalues and Positivity (continued)

Proof.

That is

$$v_i \cdot v_j = v_i^T v_j = \begin{cases} 0 & \text{for } i \neq j \\ 1 & \text{for } i = j \end{cases}.$$

For any $v \in \mathbb{R}^n$ there exist unique $\alpha_1, \dots, \alpha_n \in \mathbb{R}$ such that

$$v = \alpha_1 v_1 + \dots + \alpha_n v_n.$$

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Now

$$\begin{aligned} Q(v) &= v^T M v = v^T M (\alpha_1 v_1 + \dots + \alpha_n v_n) = \\ &= (\alpha_1 v_1 + \dots + \alpha_n v_n)^T (\lambda_1 \alpha_1 v_1 + \dots + \lambda_n \alpha_n v_n) = \lambda_1 \alpha_1^2 + \dots + \lambda_n \alpha_n^2. \end{aligned}$$

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In particular

$$Q(v_i) = v_i^T M v_i = \lambda_i,$$

$$Q(v) > 0 \text{ for any } v \neq 0 \iff \lambda_1, \dots, \lambda_n > 0,$$

$$Q(v) \geq 0 \text{ for any } v \iff \lambda_1, \dots, \lambda_n \geq 0.$$

Example

Let

$$M = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The eigenvalues are $\lambda_1 = 1 > 0$, $\lambda_2 = -1 < 0$ therefore the quadratic form $Q((x_1, x_2)) = x_1^2 - x_2^2$ is indefinite.

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The characteristic polynomial

$w_M(\lambda) = (1 - \lambda)((2 - \lambda)^2 - 4) = \lambda(1 - \lambda)(\lambda - 4)$ has non-negative roots $\lambda_1 = 0, \lambda_2 = 1, \lambda_3 = 4, \lambda_1, \lambda_2, \lambda_3 \geq 0$.

Therefore the quadratic form

$Q((x_1, x_2, x_3)) = x_1^2 + 2x_2^2 + 2x_3^2 + 4x_2x_3 = x_1^2 + 2(x_2 + x_3)^2$ is positive semidefinite.

Example (continued)

Let $A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 1 & 3 \end{bmatrix} \in M(3 \times 2; \mathbb{R})$ where $r(A) = 2$. The matrix

$$A^T A = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 & 1 \\ 2 & 1 & 3 \end{bmatrix} = \begin{bmatrix} 5 & 4 & 7 \\ 4 & 5 & 5 \\ 7 & 5 & 10 \end{bmatrix},$$

is positive semidefinite and it is not positive definite.

$$\begin{aligned} \det \begin{bmatrix} 5-\lambda & 4 & 7 \\ 4 & 5-\lambda & 5 \\ 7 & 5 & 10-\lambda \end{bmatrix} &\stackrel{c_3-2c_2}{=} \det \begin{bmatrix} 5-\lambda & 4 & -1 \\ 4 & 5-\lambda & 2\lambda-5 \\ 7 & 5 & -\lambda \end{bmatrix} \stackrel{\substack{c_1+(5-\lambda)c_3 \\ c_2+4c_3}}{=} \\ &= \det \begin{bmatrix} 0 & 0 & -1 \\ -2\lambda^2+15\lambda-21 & 7\lambda-15 & 2\lambda-5 \\ \lambda^2-5\lambda+7 & 5-4\lambda & -\lambda \end{bmatrix} = \\ &= -\det \begin{bmatrix} -2\lambda^2+15\lambda-21 & 7\lambda-15 \\ \lambda^2-5\lambda+7 & 5-4\lambda \end{bmatrix} = \\ &= -\lambda(\lambda^2-20\lambda+35). \end{aligned}$$

Example (continued)

Therefore one eigenvalue of $A^T A$ is equal to 0, and, by the Viète's formulas,

$$\lambda_1 + \lambda_2 = 20 > 0,$$

$$\lambda_1 \lambda_2 = 35 > 0,$$

the other two eigenvalues are non-negative. In fact

$$\begin{bmatrix} 5 & -1 & -3 \end{bmatrix} \begin{bmatrix} 5 & 4 & 7 \\ 4 & 5 & 5 \\ 7 & 5 & 10 \end{bmatrix} \begin{bmatrix} 5 \\ -1 \\ -3 \end{bmatrix} = 0.$$

Spectral Theorem

Proposition

Let $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^n$ be an endomorphism. If there exists an orthonormal basis \mathcal{A} of \mathbb{R}^n such that $M(\varphi)_{\mathcal{A}}^{\mathcal{A}}$ is symmetric then for any orthonormal basis \mathcal{B} of \mathbb{R}^n matrix $M(\varphi)_{\mathcal{B}}^{\mathcal{B}}$ is symmetric.

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Proof.

Let $M = M(\varphi)_{\mathcal{A}}^{\mathcal{A}}$, $N = M(\varphi)_{\mathcal{B}}^{\mathcal{B}}$. Matrix

$$Q = M(\text{id})_{\mathcal{B}}^{\mathcal{A}} = M(\text{id})_{st}^{\mathcal{A}} M(\text{id})_{\mathcal{B}}^{st},$$

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is orthogonal, i.e. $Q^{-1} = Q^T$. Because

$$N = Q^T M Q,$$

we have

$$N^T = Q^T M^T (Q^T)^T = N.$$



Spectral Theorem (continued)

Proposition

Let $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^n$ be an endomorphism such that matrix $M(\varphi)_{st}^{st}$ is symmetric. Then there exists $\mu \in \mathbb{R}$ and $v \in \mathbb{R}^n$, $v \neq \mathbf{0}$ such that $\varphi(v) = \mu v$, i.e μ is an eigenvalue of φ and v is an eigenvector for μ .

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Proof.

Let $M = M(\varphi)_{st}^{st}$ and let $w_M(\lambda) = \det(M - \lambda I_n)$ be the characteristic polynomial of φ . By the fundamental theorem of algebra there exists a complex root $\mu \in \mathbb{C}$ of w_M and a complex eigenvector $v \in \mathbb{C}^n$, i.e. $w_M(\mu) = 0$ and $Mv = \mu v$. Matrix M is real therefore $M\bar{v} = \overline{\mu v}$. Moreover

$$\bar{v}^T Mv = (M\bar{v})^T v = \overline{\mu v}^T v = \overline{\mu} \|v\|,$$

$$\bar{v}^T Mv = \bar{v}^T (Mv) = \bar{v}^T (\mu v) = \mu \|v\|.$$

This implies $\mu \in \mathbb{R}$ and since $V_{(\mu)}$ is given a system of linear equations with real coefficients one can choose $v \in \mathbb{R}^n$.

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Proposition

Let $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^n$ be an endomorphism such that matrix $M(\varphi)_{st}^{st}$ is symmetric. Then for any subspace $W \subset \mathbb{R}^n$ such that $\varphi(W) \subset W$,

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$$v^\top Mw = (Mv)^\top w = 0.$$

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Symmetric matrix $M \in M(n \times n; \mathbb{R})$ is diagonalizable.

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Let φ be an endomorphism given by $M = M(\varphi)_{st}^{st}$. Assume $W \subset \mathbb{R}^n$ is a subspace spanned by pairwise perpendicular eigenvectors of φ . Let $V = W^\perp$.

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Spectral Theorem (continued)

Corollary

For any symmetric matrix $M \in M(n \times n; \mathbb{R})$ there exists matrix $Q \in M(n \times n; \mathbb{R})$ such that $Q^{-1} = Q^T$ and the matrix

$$D = Q^T M Q,$$

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Proof.

Let $\mathcal{A} = (v_1, \dots, v_n)$ be an orthonormal basis of \mathbb{R}^n consisting of eigenvectors of M . If $Q = M(\text{id})_{\mathcal{A}}^{st}$ then the matrix $Q^{-1} M Q$ is diagonal and $Q^T Q = I_n$, i.e. $Q^{-1} = Q^T$. □

Characterization of Real Symmetric Matrices

Corollary

Let $M \in M(n \times n; \mathbb{R})$ be a real matrix. Then $M = M^T$ if and only if there exists an orthogonal matrix $Q \in M(n \times n; \mathbb{R})$ (i.e. $Q^T Q = I$) such that the matrix

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(\Rightarrow) previous corollary

(\Leftarrow) If $D = Q^T M Q$ then $M = Q D Q^T$ and since $D^T = D$

$$M^T = (Q^T)^T D^T Q^T = Q D Q^T = M.$$

Bilinear Form

Definition

Let V be a vector space. A function

$$B: V \times V \rightarrow \mathbb{R}$$

is called a **bilinear form** if

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Bilinear form B is called **symmetric** if moreover

- v) $B(v, w) = B(w, v)$ for any $v, w \in V$.

Bilinear Forms (continued)

Definition

If $B: V \times V \rightarrow \mathbb{R}$ is a bilinear form and $\mathcal{A} = (v_1, \dots, v_n)$ is a basis of V then the **matrix of bilinear form** B relative to the basis \mathcal{A} is equal to

$$M(B)_{\mathcal{A}} = [m_{ij}] \in M(n \times n; \mathbb{R}),$$

where $m_{ij} = B(v_i, v_j)$, i.e

$$M(B)_{\mathcal{A}} = \begin{bmatrix} B(v_1, v_1) & B(v_1, v_2) & \dots & B(v_1, v_n) \\ B(v_2, v_1) & B(v_2, v_2) & \dots & B(v_2, v_n) \\ \vdots & \vdots & \ddots & \vdots \\ B(v_n, v_1) & B(v_n, v_2) & \dots & B(v_n, v_n) \end{bmatrix}.$$

Bilinear Forms (continued)

Proposition

For any $v, w \in V$ and any basis \mathcal{A}

$$B(v, w) = [v]_{\mathcal{A}}^T M(B)_{\mathcal{A}} [w]_{\mathcal{A}}.$$

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Proposition

For any $v, w \in V$ and any basis \mathcal{A}

$$B(v, w) = [v]_{\mathcal{A}}^T M(B)_{\mathcal{A}} [w]_{\mathcal{A}}.$$

Proof.

Let $\mathcal{A} = (v_1, \dots, v_n)$ and let

$$v = \alpha_1 v_1 + \dots + \alpha_n v_n, w = \beta_1 v_1 + \dots + \beta_n v_n.$$

$$\begin{aligned} B(v, w) &= \sum_{i=1}^n \alpha_i \left(\sum_{j=1}^n B(v_i, w_j) \beta_j \right) = \\ &= \sum_{i=1}^n \alpha_i \left(\sum_{j=1}^n m_{ij} \beta_j \right), \end{aligned}$$

where $M(B)_{\mathcal{A}} = [m_{ij}]$.



Bilinear Forms (continued)

Corollary

If \mathcal{A}, \mathcal{B} are bases of V then for $C = M(\text{id})_{\mathcal{A}}^{\mathcal{B}}$

$$M(B)_{\mathcal{A}} = C^{\top} M(B)_{\mathcal{B}} C.$$

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If \mathcal{A}, \mathcal{B} are bases of V then for $C = M(\text{id})_{\mathcal{A}}^{\mathcal{B}}$

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Proof.

Let $M(B)_{\mathcal{A}} = M = [m_{ij}]$ and let $\mathcal{A} = (v_1, \dots, v_n)$. By the previous proposition

$$\begin{aligned}\varepsilon_i^T (C^T M(B)_{\mathcal{B}} C) \varepsilon_j &= (C \varepsilon_j)^T M(B)_{\mathcal{B}} (C \varepsilon_i) = [v_j]_{\mathcal{B}}^T M(B)_{\mathcal{B}} [v_i]_{\mathcal{B}} = \\ &= B(v_i, v_j).\end{aligned}$$

On the other hand, for any $M = [m_{ij}]$

$$\varepsilon_i^T M \varepsilon_j = m_{ij},$$

hence $C^T M(B)_{\mathcal{B}} C = M = M(B)_{\mathcal{A}}$.

Bilinear Forms (continued)

Let $B: V \times V \rightarrow \mathbb{R}$.

Corollary

If B is a symmetric bilinear form then for any basis \mathcal{A} of V

$$M(B)_{\mathcal{A}}^{\top} = M(B)_{\mathcal{A}}.$$

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If B is a symmetric bilinear form then for any basis \mathcal{A} of V

$$M(B)_{\mathcal{A}}^T = M(B)_{\mathcal{A}}.$$

If B is a bilinear form and for some basis \mathcal{A} of V

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then B is symmetric bilinear form.

Proof.

For the second claim, let $M = [m_{ij}] = M(B)_{\mathcal{A}}$ be symmetric, i.e. $M^T = M$. Then for any $v, w \in \mathbb{R}^n$

$$B(v, w) = [v]_{\mathcal{A}}^T M [w]_{\mathcal{A}} = \left([v]_{\mathcal{A}}^T M [w]_{\mathcal{A}} \right)^T = [w]_{\mathcal{A}}^T M [v]_{\mathcal{A}} = B(w, v),$$

i.e. B is symmetric.

Quadratic Forms

Let V be a vector space.

Definition

Function $Q: V \rightarrow \mathbb{R}$ is a **quadratic form** if there exist a bilinear form $B: V \times V \rightarrow \mathbb{R}$ such that $Q(v) = B(v, v)$ for any $v \in V$.

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Proposition

If $Q: V \rightarrow \mathbb{R}$ is a quadratic form then

$$B_s(v, w) = \frac{1}{2} (Q(v + w, v + w) - Q(v, v) - Q(w, w)),$$

*is a **symmetric** bilinear form such that $Q(v) = B_s(v, v)$.*

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Proof.

$$B_s(v, w) = \frac{1}{2} (B(v, w) + B(w, v)).$$



Sylvester's Criterion

Proposition

Let $Q: V \rightarrow \mathbb{R}$ be a quadratic form such that $Q(v) = B(v, v)$ where B is a symmetric bilinear form. Let $\mathcal{A} = (v_1, \dots, v_n)$ be a basis of V . Then Q is positive definite if and only if

$$\det M(B)_{\mathcal{A}_i} > 0,$$

for $i = 1, \dots, n$ where $\mathcal{A}_i = (v_1, \dots, v_i)$.

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Proof.

(\Rightarrow) The quadratic form Q restricted to $\text{lin}(v_1, \dots, v_i)$ is positive hence the matrix $M(B)_{\mathcal{A}_i}$ is symmetric diagonalizable and by the eigenvalue criterion its all eigenvalues $\lambda_1, \dots, \lambda_i > 0$ are positive. Therefore

$$\det M(B)_{\mathcal{A}_i} = \lambda_1 \cdot \dots \cdot \lambda_i > 0.$$

Note that eigenvalues depend on i .

Sylvester's Criterion (continued)

Proof.

(\Leftarrow) let $V_k = \text{lin}(v_1, \dots, v_k)$. By induction on k we prove the claim

„the quadratic form $Q|_{V_k}$ is positive definite”,

which for $k = n$ is the assertion of the Theorem.

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For $k = 1$ the claim holds since $\det M(B)_{\mathcal{A}_1} = B(v_1, v_1) > 0$.

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For $k = 2$ let $\lambda_1, \lambda_2 \in \mathbb{R}$ are eigenvalues of $M(B)_{\mathcal{A}_2}$. By Viète's formulas

$$\begin{cases} \lambda_1 + \lambda_2 &= B(v_1, v_1) + B(v_2, v_2), \\ \lambda_1 \lambda_2 &= B(v_1, v_1)B(v_2, v_2) - B(v_1, v_2)^2. \end{cases}$$

Because $\lambda_1 \lambda_2 = \det M(B)_{\mathcal{A}_2} > 0$ either

$B(v_1, v_1) < 0, B(v_2, v_2) < 0$ or $B(v_1, v_1) > 0, B(v_2, v_2) > 0$. Since $B(v_1, v_1) = \det M(B)_{\mathcal{A}_1} > 0$ the latter holds, hence $\lambda_1, \lambda_2 > 0$.

Sylvester's Criterion (continued)

Proof.

Assume that $k \geq 3$ and $\det M(B)_{\mathcal{A}_i} > 0$, for $i = 1, \dots, k$ (i.e. $Q|_{V_{k-1}}$ is positive definite) but $Q|_{V_k}$ is not positive definite.

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Therefore $M(B)_{\mathcal{A}_k}$ has at least two negative eigenvalues $\lambda_1, \lambda_2 < 0$ or a negative eigenvalue $\lambda < 0$ of multiplicity at least 2 ($\det M(B)_{\mathcal{A}_k} > 0$ is equal to the product of eigenvalues).

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In both cases there exist eigenvectors $w_1, w_2 \in V_k$ of $M(B)_{\mathcal{A}_k}$, that is

$$M(B)_{\mathcal{A}_k} [w_i]_{\mathcal{A}_k} = \lambda_i [w_i]_{\mathcal{A}_k} \text{ for } i = 1, 2,$$

and $[w_1]_{\mathcal{A}_k}^T [w_2]_{\mathcal{A}_k} = 0$ (including the case $\lambda_1 = \lambda_2 = \lambda$).

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and $[w_1]_{\mathcal{A}_k}^T [w_2]_{\mathcal{A}_k} = 0$ (including the case $\lambda_1 = \lambda_2 = \lambda$). Note that $w_1, w_2 \notin V_{k-1}$.

Sylvester's Criterion (continued)

Proof.

Let $w_1 = \alpha_1 v_1 + \dots + \alpha_k v_k$, $w_2 = \beta_1 v_1 + \dots + \beta_k v_k$ and let $v = \gamma_1 w_1 + \gamma_2 w_2 \in V_{k-1}$ where $\gamma_1 = \beta_k$, $\gamma_2 = -\alpha_k$. Then $\gamma_1, \gamma_2 \neq 0$ since $w_1, w_2 \notin V_{k-1}$. Vectors w_1, w_2 are perpendicular (i.e. linearly independent), therefore $v \neq \mathbf{0}$. Hence

$$\begin{aligned} [v]_{\mathcal{A}_k}^T M(B)_{\mathcal{A}_k} [v]_{\mathcal{A}_k} &= \\ &= \left(\gamma_1 [w_1]_{\mathcal{A}_k} + \gamma_2 [w_2]_{\mathcal{A}_k} \right)^T M(B)_{\mathcal{A}_k} \left(\gamma_1 [w_1]_{\mathcal{A}_k} + \gamma_2 [w_2]_{\mathcal{A}_k} \right) = \\ &= \lambda_1 \gamma_1^2 \| [w_1]_{\mathcal{A}_k} \|^2 + \lambda_2 \gamma_2^2 \| [w_2]_{\mathcal{A}_k} \|^2 < 0. \end{aligned}$$

On the other hand

$$[v]_{\mathcal{A}_k}^T M(B)_{\mathcal{A}_k} [v]_{\mathcal{A}_k} = Q(v) > 0,$$

because $Q|_{V_{k-1}}$ is positive definite, which yields a contradiction.

Summary

Let $M \in M(n \times n; \mathbb{R})$ be a symmetric matrix. The following are equivalent

- i) $x^T M x \geq 0$ (matrix M is positive semidefinite),
- ii) $\min\{\lambda \mid \lambda \text{ is an eigenvalue of } M\} \geq 0$,
- iii) $\min\{x^T M x \in \mathbb{R} \mid \|x\| = 1\} \geq 0$,
- iv) all principal minors of M are non-negative,
- v) there exists a matrix $N \in M(n \times n; \mathbb{R})$ such that $M = N^T N$.

Summary (continued)

Let $M \in M(n \times n; \mathbb{R})$ be a symmetric matrix. The following are equivalent

- i) $x^T M x > 0$ for $x \neq \mathbf{0}$ (matrix M is positive definite),
- ii) $\min\{\lambda \mid \lambda \text{ is an eigenvalue of } M\} > 0$,
- iii) $\min\{x^T M x \in \mathbb{R} \mid \|x\| = 1\} > 0$,
- iv) all leading principal minors of M are positive,
- v) there exists a non-singular (i.e. $\det N \neq 0$) matrix $N \in M(n \times n; \mathbb{R})$ such that $M = N^T N$.

Interlacing Eigenvalues

Theorem

If $M \in M(n \times n; \mathbb{R})$ is a symmetric matrix, i.e. $M = M^T$. Let M_i denote the top left i -by- i submatrix of M . Fix $m < n$. Let $\lambda_1, \dots, \lambda_m$ denote the eigenvalues of M_m and μ_1, \dots, μ_{m+1} denote the eigenvalues of M_{m+1} . Then

$$\mu_1 \leq \lambda_1 \leq \mu_2 \leq \lambda_2 \leq \mu_3 \leq \dots \leq \lambda_m \leq \mu_{m+1}.$$

Proof.

Omitted.



Hessian Matrix

Definition

Let $f: U \rightarrow \mathbb{R}$, $U \subset \mathbb{R}^k$, be a function of class \mathcal{C}^2 on the open set U . **Hessian matrix** at $x_0 \in U$ is the symmetric matrix

$H_f(x_0) = H(x_0) \in M(k \times k; \mathbb{R})$ given by

$$H_f(x_0) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2}(x_0) & \frac{\partial^2 f}{\partial x_1 \partial x_2}(x_0) & \frac{\partial^2 f}{\partial x_1 \partial x_3}(x_0) & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_k}(x_0) \\ \frac{\partial^2 f}{\partial x_2 \partial x_1}(x_0) & \frac{\partial^2 f}{\partial x_2^2}(x_0) & \frac{\partial^2 f}{\partial x_2 \partial x_3}(x_0) & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_k}(x_0) \\ \frac{\partial^2 f}{\partial x_3 \partial x_1}(x_0) & \frac{\partial^2 f}{\partial x_3 \partial x_2}(x_0) & \frac{\partial^3 f}{\partial x_3^3}(x_0) & \cdots & \frac{\partial^2 f}{\partial x_3 \partial x_k}(x_0) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_k \partial x_1}(x_0) & \frac{\partial^2 f}{\partial x_k \partial x_2}(x_0) & \frac{\partial^2 f}{\partial x_k \partial x_3}(x_0) & \cdots & \frac{\partial^2 f}{\partial x_k^2}(x_0) \end{bmatrix}.$$

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Remark

If f is not of class \mathcal{C}^2 the matrix $H_f(x_0)$ may not be symmetric.

Local Minima or Maxima of a Multivariate Function

Theorem

Let $f: U \rightarrow \mathbb{R}$, $U \subset \mathbb{R}^k$ be a function of class \mathcal{C}^2 on the open set U . If $x_0 \in U$ is a **critical point** of function f , i.e.

$$f'(x_0) = \left(\frac{\partial f}{\partial x_1}(x_0), \dots, \frac{\partial f}{\partial x_k}(x_0) \right) = \mathbf{0},$$

and the Hessian matrix $H(x_0)$ is negative (respectively, positive) definite, then f has strict local maximum (respectively strict local minimum) at the point $x_0 \in U$.

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and the Hessian matrix $H(x_0)$ is negative (respectively, positive) definite, then f has strict local maximum (respectively strict local minimum) at the point $x_0 \in U$.

If the matrix $H(x_0)$ is indefinite then f has no local extremum at x_0 (the point x_0 is so called **saddle point**).

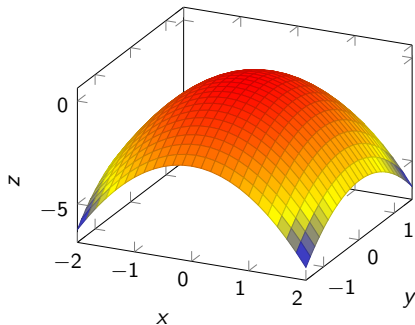
Proof.

Analysis course (use multivariate Taylor formula).



Example – Local Maximum

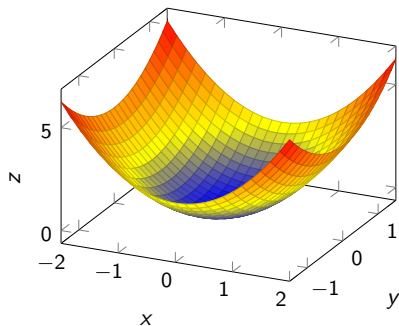
graph of the function $f(x, y) = -x^2 - y^2$



$$H_f(0,0) = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix} \text{ negative definite}$$

Example – Local Minimum

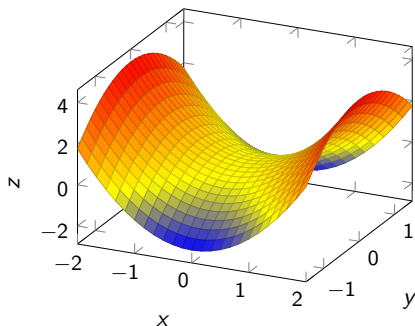
graph of the function $f(x, y) = x^2 + y^2$



$$H_f(0,0) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \text{ positive definite}$$

Example – Saddle Point – No Local Extremum

graph of the function $f(x, y) = x^2 - y^2$



$$H_f(0,0) = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix} \text{ indefinite}$$

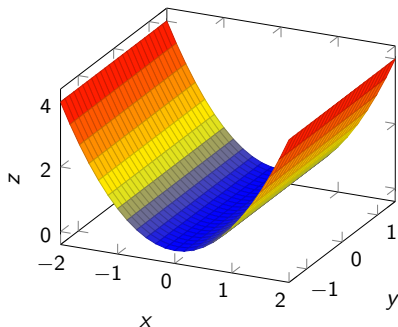
Local Minima or Maxima of a Multivariate Function (continued)

Remark

If the matrix $H(x_0)$ is positive semidefinite or negative semidefinite then the function f has at x_0 local minimum or local maximum or a saddle point (the criterion is indecisive).

Example – Hessian Matrix Positive Semidefinite – Weak Local Minimum

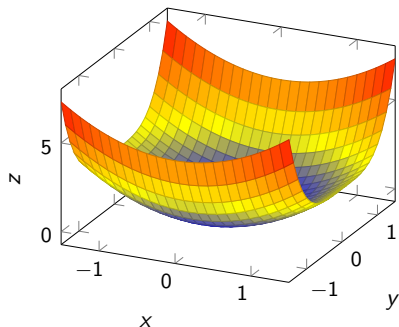
graph of the function $f(x,y) = x^2$



$$H_f(0,0) = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} \text{ positive semidefinite}$$

Example – Hessian Matrix Positive Semidefinite – Strict Local Minimum

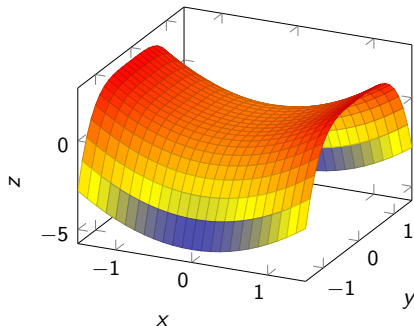
graph of the function $f(x, y) = x^2 + y^4$



$$H_f(0,0) = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} \text{ positive semidefinite}$$

Example – Hessian Matrix Positive Semidefinite – Saddle Point

graph of the function $f(x, y) = x^2 - y^4$



$$H_f(0,0) = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} \text{ positive semidefinite}$$

Square Root of a Positive Semidefinite Matrix

Find a matrix $X \in M(2 \times 2; \mathbb{R})$ such that

$$X^2 = \begin{bmatrix} 5 & -4 \\ -4 & 5 \end{bmatrix} = A.$$

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It can be checked that

$$A = Q^T \begin{bmatrix} 1 & 0 \\ 0 & 9 \end{bmatrix} Q,$$

where

$$Q = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}.$$

Square Root of a Positive Semidefinite Matrix (continued)

$$X_1 = Q^T \begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix} Q = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix},$$

$$X_2 = Q^T \begin{bmatrix} -1 & 0 \\ 0 & 3 \end{bmatrix} Q = \begin{bmatrix} 1 & -2 \\ -2 & 1 \end{bmatrix},$$

$$X_3 = Q^T \begin{bmatrix} 1 & 0 \\ 0 & -3 \end{bmatrix} Q = \begin{bmatrix} -1 & 2 \\ 2 & -1 \end{bmatrix},$$

$$X_4 = Q^T \begin{bmatrix} 1 & 0 \\ 0 & -3 \end{bmatrix} Q = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}.$$

Multivariate Gaussian Distribution

The probability density function of multivariate n -dimensional Gaussian distribution is given by

$$p(x \mid \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{n}{2}}} \frac{1}{(\det \Sigma)^{\frac{1}{2}}} e^{-\frac{1}{2}(x-\mu)^{\top} \Sigma^{-1} (x-\mu)},$$

where $x \in \mathbb{R}^n$ for some fixed $\mu \in \mathbb{R}^n$ and $\Sigma \in M(n \times n; \mathbb{R})$ a symmetric positive definite matrix.

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where $x \in \mathbb{R}^n$ for some fixed $\mu \in \mathbb{R}^n$ and $\Sigma \in M(n \times n; \mathbb{R})$ a symmetric positive definite matrix. There exists an orthogonal matrix $Q \in M(n \times n; \mathbb{R})$ (i.e. $QQ^{\top} = Q^{\top}Q = I$) such that

$$Q^{\top} \Sigma Q = \begin{bmatrix} \sigma_1^2 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \cdots & \sigma_n^2 \end{bmatrix},$$

where $\sigma_1, \dots, \sigma_n > 0$, $Q = [v_1 \ v_2 \ \cdots \ v_n]$ and $\mathcal{B} = (v_1, v_2, \dots, v_n)$ is an orthonormal basis of \mathbb{R}^n .

Multivariate Gaussian Distribution (continued)

Then if

$$x = \sum_{i=1}^n x_i v_i,$$

(i.e. $[x]_{\mathcal{B}} = [x_1 \ x_2 \ \cdots \ x_n]^T$) and

$$\mu = (\mu_1, \mu_2, \dots, \mu_n),$$

then

$$p(x \mid \mu, \Sigma) = \prod_{i=1}^n \frac{1}{(2\pi\sigma_i^2)^{\frac{1}{2}}} e^{-\frac{(x_i - \mu_i)^2}{2\sigma_i^2}},$$

i.e., it is a product of one-dimensional Gaussian probability density functions.

Multivariate Gaussian Distribution – Example

Let

$$\Sigma = \begin{bmatrix} \frac{5}{2} & -\frac{3}{2} \\ -\frac{3}{2} & \frac{5}{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}^T \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix},$$

$$\Sigma^{-1} = \begin{bmatrix} \frac{5}{8} & \frac{3}{8} \\ \frac{3}{8} & \frac{5}{8} \end{bmatrix},$$

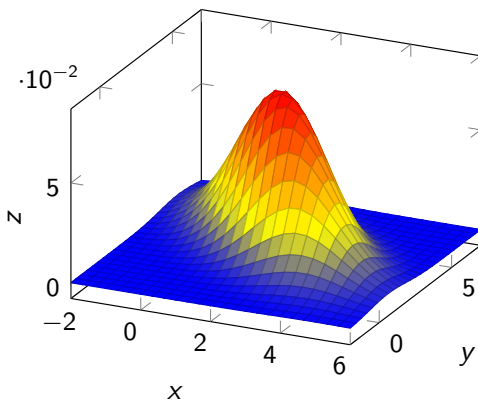
$$\mu = (2, 3), \quad v_1 = \frac{1}{\sqrt{2}}(1, 1), \quad v_2 = \frac{1}{\sqrt{2}}(1, -1),$$

then

$$p((x_1, x_2) \mid \mu, \Sigma) = \frac{1}{2\pi} \frac{1}{2} e^{-\frac{1}{16}(5(x_1-2)^2 + 6(x_1-2)(x_2-3) + 5(x_2-3)^2)},$$

$$p(x_1 v_1 + x_2 v_2 \mid \mu, \Sigma) = \frac{1}{(2\pi)^{\frac{1}{2}}} e^{-\frac{(x_1-2)^2}{2}} \frac{1}{2(2\pi)^{\frac{1}{2}}} e^{-\frac{(x_2-3)^2}{8}},$$

Multivariate Gaussian Distribution – Example



probability density functions for $\Sigma = \frac{1}{2} \begin{bmatrix} 5 & -3 \\ -3 & 5 \end{bmatrix}$, $\mu = (2, 3)$

Inner product

Definition

Inner product space V is a vector space V over \mathbb{C} or \mathbb{R} , with a function

$$\langle \cdot, \cdot \rangle: V \times V \rightarrow \mathbb{C},$$

such that

i) $\langle v, w \rangle = \overline{\langle w, v \rangle}$ for any $v, w \in V$,

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 - a) $\langle v, w + w' \rangle = \langle v, w \rangle + \langle v, w' \rangle$,

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 - b) $\langle v, \alpha w \rangle = \alpha \langle v, w \rangle$
- iii) $\langle v, v \rangle > 0$ for any $v \neq \mathbf{0}$.

Example

Example

The vector space $V = \mathbb{C}^n$ with

$$\langle v, w \rangle = \sum_{j=1}^n \overline{v_j} w_j = \overline{v}^T w = v^* w,$$

for any $v = (v_1, \dots, v_n)$, $w = (w_1, \dots, w_n) \in \mathbb{C}^n$ is the standard inner product space

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Example

The vector space $V = \mathcal{C}([a, b]; \mathbb{C})$ of continuous functions

$$\langle f, g \rangle = \int_a^b w(x) \overline{f(x)} g(x) dx,$$

where w is a fixed **weight function** $w \in V$ such that $w(x) \in \mathbb{R}$, $w(x) > 0$ for $x \in (a, b)$ is an inner product space.

Norm

Let V be an inner product space.

Definition

Norm of vector $v \in V$ is equal to

$$\|v\| = \sqrt{\langle v, v \rangle}.$$

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If V is complete as a metric space induced by the norm it is called a Hilbert space.

Adjoint Transformation

Proposition

Let V and W be inner product spaces. For any linear transformation $\varphi: V \rightarrow W$ there exists a unique linear transformation $\varphi^: W \rightarrow V$ such that*

$$\langle \varphi(v), w \rangle_W = \langle v, \varphi^*(w) \rangle_V.$$

Adjoint Transformation (continued)

Proof.

The inner products induce isomorphisms $V \simeq V^*$ and $W \simeq W^*$ because the linear transformations are monomorphisms hence isomorphisms (since the product is positive definite),

$$V \ni v \mapsto \langle v, \cdot \rangle \in V^*,$$

$$W \ni w \mapsto \langle w, \cdot \rangle \in W^*.$$

These isomorphisms induce an isomorphism

$$\text{Hom}(V, W) = V^* \otimes W \simeq V \otimes W^* \simeq W^* \otimes V = \text{Hom}(W, V),$$

and φ^* is the image of φ under this isomorphism. □

Adjoint Transformation (continued)

Proof.

Let

$$\varphi = \alpha \otimes t,$$

where $\alpha \in V^*$, $t \in W$. Let $s_\alpha \in V$ be a vector such that

$$\alpha(\cdot) = \langle s_\alpha, \cdot \rangle,$$

(i.e. vector corresponding to α under isomorphism $V \simeq V^*$). By definition

$$\alpha^* = \langle t, \cdot \rangle \otimes s_\alpha.$$

Then for any $v \in V$, $w \in W$

$$\langle \varphi(v), w \rangle = \langle \alpha(v)t, w \rangle = \overline{\alpha(v)} \langle t, w \rangle.$$

On the other hand

$$\langle v, \varphi^*(w) \rangle = \langle v, \langle t, w \rangle s_\alpha \rangle = \langle t, w \rangle \langle v, s_\alpha \rangle = \langle t, w \rangle \overline{\alpha(v)}.$$

Adjoint Transformation (continued)

Proposition

Let $\varphi: \mathbb{C}^n \rightarrow \mathbb{C}^n$ be a linear transformation where \mathbb{C}^n is a standard inner product space (domain and codomain). If $A = M_{st}^{st}(\varphi)$ then

$$A^* = \overline{A}^T = M_{st}^{st}(\varphi^*),$$

where

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Adjoint Transformation (continued)

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where

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Proof.

For any $v = (v_1, \dots, v_n)$, $w = (w_1, \dots, w_n) \in \mathbb{C}^n$

$$\langle Av, w \rangle = (\overline{A} \overline{v})^T w = \overline{v}^T (\overline{A}^T w) = \overline{v}^T A^* w = \langle v, A^* w \rangle.$$



Normal, Unitary, Hermitian and Skew-Hermitian Matrix

Definition

Matrix $A \in M(n \times n; \mathbb{C})$ is **normal** if

$$A^*A = AA^*.$$

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Definition

Matrix $H \in M(n \times n; \mathbb{C})$ is **Hermitian** if

$$H = H^*.$$

Matrix $H \in M(n \times n; \mathbb{C})$ is **skew-Hermitian** if

$$H = -H^*.$$

Normal, Unitary, Hermitian and Skew-Hermitian Matrix (continued)

Proposition

Unitary, Hermitian and skew-Hermitian matrices are normal.

Normal Transformation

Let V be an inner product space.

Definition

Endomorphism (linear transformation)

$$\varphi: V \rightarrow V,$$

is **normal** if

$$\varphi \circ \varphi^* = \varphi^* \circ \varphi.$$

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Endomorphism φ is normal if and only if the matrix $M_{\mathcal{A}}^{\mathcal{A}}(\varphi)$ is normal for any (some) orthonormal basis \mathcal{A} of V .

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Proof.

Exercise.



Normal Matrix is Unitary Diagonalizable

Proposition

Let $A \in M(n \times n; \mathbb{C})$ be normal matrix. Then there exists a unitary matrix $U \in M(n \times n; \mathbb{C})$ such that the matrix

$$U^*AU = U^{-1}AU,$$

is diagonal.

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is diagonal.

Proof.

Let $\lambda \in \mathbb{C}$, $v \in \mathbb{C}^n$. Then

$$\begin{aligned}\|Av - \lambda v\|^2 &= \langle Av, Av \rangle - \langle \lambda v, Av \rangle - \langle Av, \lambda v \rangle + \langle \lambda v, \lambda v \rangle = \\ &= \langle v, A^*Av \rangle - \langle A^*v, \bar{\lambda}v \rangle - \langle \bar{\lambda}v, A^*v \rangle + \langle \bar{\lambda}v, \bar{\lambda}v \rangle = \\ &= \langle v, AA^*v \rangle - \langle A^*v, \bar{\lambda}v \rangle - \langle \bar{\lambda}v, A^*v \rangle + \langle \bar{\lambda}v, \bar{\lambda}v \rangle = \\ &= \|A^*v - \bar{\lambda}v\|^2.\end{aligned}$$

Therefore $v \in \mathbb{C}^n$ is an eigenvector of A if and only if it is an eigenvector of A^* (and the corresponding eigenvalues are conjugated).

Normal Matrix is Unitary Diagonalizable (continued)

Proof.

Let $\lambda \in \mathbb{C}$ be an eigenvalue of A and let $v \in \mathbb{C}^n$ be a corresponding eigenvector of norm 1. Let

$$V = \text{lin}(v)^\perp = \{w \in W \mid \langle v, w \rangle = 0\}.$$

Then

$$AV \subset V,$$

since for $w \in V$

$$\langle v, Aw \rangle = \langle A^* v, w \rangle = \langle \bar{\lambda} v, w \rangle = 0.$$

The endomorphism $A|_V$ is normal (since $(\varphi|_V)^* = (\varphi^*)|_V$) and by the induction the theorem holds. The unitary matrix $U \in M(n \times n; \mathbb{C})$ has in columns normalized (i.e. of length 1) eigenvectors obtained by the above procedure. □

Characterization of Complex Normal, Unitary, Hermitian and Skew-Hermitian Matrices

Let $A \in M(n \times n; \mathbb{C})$ be a matrix with (possibly repeating) eigenvalues $\lambda_1, \dots, \lambda_n \in \mathbb{C}$. Let $D = \text{diag}(\lambda_1, \dots, \lambda_n) \in M(n \times n; \mathbb{C})$ be a diagonal matrix with complex numbers $\lambda_1, \dots, \lambda_n \in \mathbb{C}$ on the diagonal.

Proposition

Then

A is normal \Leftrightarrow

\Leftrightarrow there exists unitary matrix $U \in M(n \times n; \mathbb{C})$ such that $U^*AU = D$.

Moreover

- i) matrix A is unitary $\Leftrightarrow |\lambda_j| = 1$ for $j = 1, \dots, n$,
- ii) matrix A is Hermitian $\Leftrightarrow \lambda_j \in \mathbb{R}$ for $j = 1, \dots, n$,
- iii) matrix A is skew-Hermitian $\Leftrightarrow \lambda_j \in \sqrt{-1}\mathbb{R}$ for $j = 1, \dots, n$,

Characterization of Complex Normal, Unitary, Hermitian and Skew-Hermitian Matrices (continued)

Proof.

Easy exercise. Respectively, one has

i) $D^* = D^{-1},$

ii) $D^* = D,$

iii) $D^* = -D.$



Normal, Orthogonal, Symmetric and Skew-Symmetric Matrix

Definition

Matrix $A \in M(n \times n; \mathbb{R})$ is **normal** if

$$A^T A = A A^T.$$

Normal, Orthogonal, Symmetric and Skew-Symmetric Matrix

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$$Q^T Q = Q Q^T = I_n.$$

Definition

Matrix $H \in M(n \times n; \mathbb{R})$ is **symmetric** if

$$H = H^T.$$

Matrix $H \in M(n \times n; \mathbb{R})$ is **skew-symmetric** if

$$H = -H^T.$$

Normal, Orthogonal, Symmetric and Skew-Symmetric Matrix (continued)

Proposition

Orthogonal, symmetric and skew-symmetric real matrices are normal.

Characterization of Real Normal Matrices

Proposition

Let $A \in M(n \times n; \mathbb{R})$ be a normal matrix. Then

- i) λ is an eigenvalue of $A \iff \overline{\lambda}$ is an eigenvalue of A ,*
- ii) $v = \operatorname{Re} v + i \operatorname{Im} v$ is an eigenvector for the eigenvalue λ of $A \iff \overline{v} = \operatorname{Re} v - i \operatorname{Im} v$ is an eigenvector for the eigenvalue $\overline{\lambda}$ of A .*

Characterization of Real Normal Matrices (continued)

Proof.

The characteristic polynomial of A has real coefficients hence its strictly complex roots form pairs $\lambda, \bar{\lambda}$. Let $\lambda = a + bi$ where $a, b \in \mathbb{R}$.

$$\begin{aligned} Av = \lambda v &\Leftrightarrow A(\operatorname{Re} v + i \operatorname{Im} v) = (a + bi)(\operatorname{Re} v + i \operatorname{Im} v) \Leftrightarrow \\ &\Leftrightarrow \begin{cases} A \operatorname{Re} v = a \operatorname{Re} v - b \operatorname{Im} v \\ A \operatorname{Im} v = b \operatorname{Re} v + b \operatorname{Im} v \end{cases}, \end{aligned}$$

where the right-hand side remains invariant under changing the sign of b and $\operatorname{Im} v$. □

Characterization of Real Normal Matrices (continued)

Proposition

Let $A \in M(n \times n; \mathbb{R})$ be a normal matrix. Let $v, w \in \mathbb{C}^n$ be two complex eigenvectors corresponding, respectively, to eigenvalues λ and μ of A . Assume $\bar{\lambda} \neq \mu$. Then

$$(\operatorname{Re} v) \cdot (\operatorname{Re} w) = (\operatorname{Im} v) \cdot (\operatorname{Im} w) = (\operatorname{Re} v) \cdot (\operatorname{Im} w) = (\operatorname{Im} v) \cdot (\operatorname{Re} w) = 0.$$

Characterization of Real Normal Matrices (continued)

Proposition

Let $A \in M(n \times n; \mathbb{R})$ be a normal matrix. Let $v, w \in \mathbb{C}^n$ be two complex eigenvectors corresponding, respectively, to eigenvalues λ and μ of A . Assume $\bar{\lambda} \neq \mu$. Then

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Proof.

Assume $w \notin \mathbb{R}$. Then w, \bar{w} are eigenvectors of A , both unitary orthogonal to v .

$$\begin{cases} \langle \operatorname{Re} v + i \operatorname{Im} v, \operatorname{Re} w + i \operatorname{Im} w \rangle = 0 \\ \langle \operatorname{Re} v + i \operatorname{Im} v, \operatorname{Re} w - i \operatorname{Im} w \rangle = 0 \end{cases} \Leftrightarrow$$

$$\Leftrightarrow \begin{cases} (\langle \operatorname{Re} v, \operatorname{Re} w \rangle + \langle \operatorname{Im} v, \operatorname{Im} w \rangle) + i(\langle \operatorname{Im} v, \operatorname{Re} w \rangle - \langle \operatorname{Re} v, \operatorname{Im} w \rangle) = 0 \\ (\langle \operatorname{Re} v, \operatorname{Re} w \rangle - \langle \operatorname{Im} v, \operatorname{Im} w \rangle) + i(\langle \operatorname{Im} v, \operatorname{Re} w \rangle + \langle \operatorname{Re} v, \operatorname{Im} w \rangle) = 0 \end{cases}$$

Characterization of Real Normal Matrices (continued)

Proof.

If $\lambda, \mu \in \mathbb{R}$ then they are different, and $(\operatorname{Re} v) \cdot (\operatorname{Re} w) = 0$ since $v = \operatorname{Re} v, w = \operatorname{Re} w$ are real and unitary orthogonal.

Characterization of Real Normal Matrices (continued)

Proof.

If $\lambda, \mu \in \mathbb{R}$ then they are different, and $(\operatorname{Re} v) \cdot (\operatorname{Re} w) = 0$ since $v = \operatorname{Re} v, w = \operatorname{Re} w$ are real and unitary orthogonal. If $\lambda \in \mathbb{R}$ and $\mu \notin \mathbb{R}$ then the above proof works as well. □

Characterization of Real Normal Matrices (continued)

Proof.

If $\lambda, \mu \in \mathbb{R}$ then they are different, and $(\operatorname{Re} v) \cdot (\operatorname{Re} w) = 0$ since $v = \operatorname{Re} v, w = \operatorname{Re} w$ are real and unitary orthogonal. If $\lambda \in \mathbb{R}$ and $\mu \notin \mathbb{R}$ then the above proof works as well. \square

Corollary

If $v, w \in \mathbb{C}$ are complex eigenvectors for the strictly complex eigenvalue λ , and $\langle v, w \rangle = 0$ (i.e. unitary orthogonal) then

$$(\operatorname{Re} v) \cdot (\operatorname{Re} w) = (\operatorname{Im} v) \cdot (\operatorname{Im} w) = (\operatorname{Re} v) \cdot (\operatorname{Im} w) = (\operatorname{Im} v) \cdot (\operatorname{Re} w) = 0.$$

Characterization of Real Normal Matrices (continued)

Proposition

*Let $A \in M(n \times n; \mathbb{R})$ be a normal matrix. Let $v \in \mathbb{C}^n$ be a **unit** complex eigenvector corresponding to a strictly complex eigenvalue $\lambda \notin \mathbb{R}$. Then*

$$(\operatorname{Re} v) \cdot (\operatorname{Im} v) = 0,$$

and

$$\|\operatorname{Re} v\| = \|\operatorname{Im} v\| = \frac{1}{\sqrt{2}}.$$

Characterization of Real Normal Matrices (continued)

Proposition

Let $A \in M(n \times n; \mathbb{R})$ be a normal matrix. Let $v \in \mathbb{C}^n$ be a **unit** complex eigenvector corresponding to a strictly complex eigenvalue $\lambda \notin \mathbb{R}$. Then

$$(\operatorname{Re} v) \cdot (\operatorname{Im} v) = 0,$$

and

$$\|\operatorname{Re} v\| = \|\operatorname{Im} v\| = \frac{1}{\sqrt{2}}.$$

Proof.

Then \bar{v} is a unit eigenvector, unitary orthogonal to v

$$\begin{aligned} 0 &= \langle \operatorname{Re} v + i \operatorname{Im} v, \operatorname{Re} v - i \operatorname{Im} v \rangle = \\ &= (\langle \operatorname{Re} v, \operatorname{Re} v \rangle - \langle \operatorname{Im} v, \operatorname{Im} v \rangle) + 2i \langle \operatorname{Re} v, \operatorname{Im} v \rangle, \end{aligned}$$

moreover

$$1 = \|v\|^2 = \|\operatorname{Re} v\|^2 + \|\operatorname{Im} v\|^2.$$

Characterization of Real Normal Matrices (continued)

Corollary

Let $A \in M(n \times n; \mathbb{R})$ be a normal matrix. Let $\mu_1, \dots, \mu_m \in \mathbb{R}$ be (possibly repeating) real eigenvalues of A . Let $\lambda_1, \overline{\lambda_1}, \lambda_2, \overline{\lambda_2}, \dots, \lambda_k, \overline{\lambda_k} \in \mathbb{C}$ be (possibly repeating) strictly complex eigenvalues of A , where $\alpha_j = a_j + ib_j$ for $j = 1, \dots, k$. Let $u_1, \dots, u_m, v_1, \overline{v_1}, v_2, \overline{v_2}, \dots, v_k, \overline{v_k} \in \mathbb{C}^n$ be the corresponding unitary orthonormal basis of \mathbb{C}^n , consisting of the corresponding eigenvectors, such that $u_j = \operatorname{Re} u_j$ for $j = 1, \dots, m$. Then

$$\mathcal{A} = (u_1, \dots, u_k,$$

$$\sqrt{2} \operatorname{Re} v_1, \sqrt{2} \operatorname{Im} v_1, \sqrt{2} \operatorname{Re} v_2, \sqrt{2} \operatorname{Im} v_2, \dots, \sqrt{2} \operatorname{Re} v_k, \sqrt{2} \operatorname{Im} v_k),$$

is an real orthogonal basis of \mathbb{R}^n .

Characterization of Real Normal Matrices (continued)

Corollary

Moreover, if $Q = M(\text{id})_{\mathcal{A}}^{st}$ then $Q \in M(n \times n; \mathbb{R})$ is an (real) orthogonal matrix (i.e. $Q^T Q = Q Q^T = I$) and

$$Q^T A Q = \begin{bmatrix} \mu_1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \mu_2 & \cdots & 0 & 0 & 0 & 0 & 0 & & 0 & 0 \\ \vdots & & \ddots & & & & & & & \vdots & \vdots \\ 0 & & & \mu_m & & & & & & 0 & 0 \\ 0 & & & & a_1 & b_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & & & & -b_1 & a_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & & & & 0 & 0 & a_2 & b_2 & & 0 & 0 \\ 0 & & & & 0 & 0 & -b_2 & a_2 & & 0 & 0 \\ \vdots & & & & \vdots & \vdots & & & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & & 0 & 0 & 0 & 0 & \cdots & a_k & b_k \\ 0 & 0 & 0 & & 0 & 0 & 0 & 0 & \cdots & -b_k & a_k \end{bmatrix}.$$

Characterization of Real Orthogonal Matrices (continued)

Corollary

Matrix $A \in M(n \times n; \mathbb{R})$ is orthogonal if and only if there exists an orthogonal matrix $Q \in M(n \times n; \mathbb{R})$ and numbers $\varphi_1, \dots, \varphi_k \in \mathbb{R}$ such that

$$Q^T A Q = \begin{bmatrix} \pm 1 & 0 & \cdots & 0 & & 0 & 0 & & 0 & 0 & \cdots & & 0 & 0 \\ 0 & \pm 1 & & & & 0 & 0 & & 0 & 0 & & & 0 & 0 \\ \vdots & & \ddots & & & & & & & & & & \vdots & \vdots \\ 0 & & & \pm 1 & & & & & & & & & 0 & 0 \\ 0 & & & & \cos \varphi_1 & \sin \varphi_1 & 0 & 0 & \cdots & & 0 & 0 & 0 & 0 \\ 0 & & & & -\sin \varphi_1 & \cos \varphi_1 & 0 & 0 & \cdots & & 0 & 0 & 0 & 0 \\ 0 & & & & 0 & 0 & \cos \varphi_2 & \sin \varphi_2 & & & 0 & 0 & 0 & 0 \\ 0 & & & & 0 & 0 & -\sin \varphi_2 & \cos \varphi_2 & & & 0 & 0 & 0 & 0 \\ \vdots & & & & \vdots & \vdots & & & \ddots & & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & & 0 & 0 & 0 & 0 & \cdots & \cos \varphi_k & \sin \varphi_k & & 0 & 0 \\ 0 & 0 & 0 & & 0 & 0 & 0 & 0 & \cdots & -\sin \varphi_k & \cos \varphi_k & & 0 & 0 \end{bmatrix}.$$

Characterization of Real Symmetric Matrices (continued)

Corollary

Matrix $A \in M(n \times n; \mathbb{R})$ is symmetric if and only if there exists an orthogonal matrix $Q \in M(n \times n; \mathbb{R})$ and numbers $\mu_1, \dots, \mu_n \in \mathbb{R}$ such that

$$Q^T A Q = \begin{bmatrix} \mu_1 & & 0 \\ & \ddots & \\ 0 & & \mu_n \end{bmatrix}.$$

Characterization of Real Skew-Symmetric Normal Matrices

Corollary

Matrix $A \in M(n \times n; \mathbb{R})$ is skew-symmetric if and only if there exists an orthogonal matrix $Q \in M(n \times n; \mathbb{R})$ and numbers $b_1, \dots, b_k \in \mathbb{R}$ such that

$$Q^T A Q = \begin{bmatrix} 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & & & 0 & 0 & 0 & 0 & & 0 & 0 \\ \vdots & & \ddots & & & & & & & \vdots & \vdots \\ 0 & & & 0 & & & & & & 0 & 0 \\ 0 & & & & 0 & b_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & & & & -b_1 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & & & & 0 & 0 & 0 & b_2 & & 0 & 0 \\ 0 & & & & 0 & 0 & -b_2 & 0 & & 0 & 0 \\ \vdots & & & & \vdots & \vdots & & & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & & 0 & 0 & 0 & 0 & \cdots & 0 & b_k \\ 0 & 0 & 0 & & 0 & 0 & 0 & 0 & \cdots & -b_k & 0 \end{bmatrix}.$$

Example

Let

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}.$$

Then

$$A^T A = A A^T = \begin{bmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{bmatrix}.$$

Moreover

$$w_A(x) = \det(A - xI) = -x^3 + 3x^2 - 3x + 2 = -(x-2)(x^2 - x + 1),$$

therefore

$$\mu = 2, \quad \lambda = \frac{1 + i\sqrt{3}}{2} = e^{\frac{i\pi}{3}}, \quad \bar{\lambda} = \frac{1 - i\sqrt{3}}{2} = e^{-\frac{i\pi}{3}}.$$

It can be checked that

$$V_{(\mu)} = \text{lin}((1, 1, 1)), \quad V_{(\lambda)} = \text{lin}((1, \lambda^2, -\lambda)), \quad V_{(\bar{\lambda})} = \text{lin}((1, -\lambda, \lambda^2)),$$

(note that $\lambda^3 + 1 = 0$, $\lambda^2 = \lambda - 1$, $\bar{\lambda} = \frac{1}{\lambda} = -\lambda^2$).

Example (continued)

Since

$$|(1, 1, 1)| = |(1, \lambda^2, -\lambda)| = |(1, -\lambda, \lambda^2)| = \sqrt{3},$$

we have

$$u_1 = \frac{1}{\sqrt{3}}(1, 1, 1),$$

$$v_1 = \frac{1}{\sqrt{3}}(1, \lambda^2, -\lambda),$$

$$\bar{v}_1 = \frac{1}{\sqrt{3}}(1, -\lambda, \lambda^2).$$

If

$$U = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \\ 1 & \lambda^2 & -\lambda \\ 1 & -\lambda & \lambda^2 \end{bmatrix},$$

Then

$$U^* U = U U^* = I.$$

Example (continued)

If

$$D = \begin{bmatrix} 2 & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \bar{\lambda} \end{bmatrix} = \begin{bmatrix} 2 & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & -\lambda^2 \end{bmatrix},$$

then

$$UDU^* = A,$$

i.e.

$$\begin{aligned} \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \\ 1 & \lambda^2 & -\lambda \\ 1 & -\lambda & \lambda^2 \end{bmatrix} \begin{bmatrix} 2 & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & -\lambda^2 \end{bmatrix} \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \\ 1 & -\lambda & \lambda^2 \\ 1 & \lambda^2 & -\lambda^2 \end{bmatrix} = \\ = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}. \end{aligned}$$

Example (continued)

Let

$$u_1 = v_1 = \frac{1}{\sqrt{3}}(1, 1, 1),$$

$$u_2 = \sqrt{2} \operatorname{Re} v_1 = \frac{\sqrt{2}}{\sqrt{3}} \left(1, -\frac{1}{2}, -\frac{1}{2} \right),$$

$$u_3 = \sqrt{2} \operatorname{Im} v_1 = \frac{\sqrt{2}}{\sqrt{3}} \left(0, \frac{\sqrt{3}}{2}, -\frac{\sqrt{3}}{2} \right).$$

If

$$Q = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & \sqrt{2} & 0 \\ 1 & -\frac{1}{\sqrt{2}} & \frac{\sqrt{6}}{2} \\ 1 & -\frac{1}{\sqrt{2}} & -\frac{\sqrt{6}}{2} \end{bmatrix},$$

then

$$Q^T Q = Q Q^T = I.$$

Example (continued)

Moreover, let

$$B = \begin{bmatrix} 2 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix}.$$

Then

$$QBQ^T = A,$$

i.e.

$$\begin{aligned} \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & \sqrt{2} & 0 \\ 1 & -\frac{1}{\sqrt{2}} & \frac{\sqrt{6}}{2} \\ 1 & -\frac{1}{\sqrt{2}} & -\frac{\sqrt{6}}{2} \end{bmatrix} \begin{bmatrix} 2 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{bmatrix} \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 0 \\ \sqrt{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ 0 & \frac{\sqrt{6}}{2} & -\frac{\sqrt{6}}{2} \end{bmatrix} = \\ = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}. \end{aligned}$$

Rayleigh Quotient

Definition

For any matrix $M \in M(n \times n; \mathbb{C})$ and any vector $x \in \mathbb{C}^n, x \neq \mathbf{0}$, the **Rayleigh quotient** $R(M, x)$ is equal to

$$R(M, x) = \frac{x^* M x}{x^* x}.$$

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$$R(M, x) = \frac{x^* M x}{x^* x}.$$

Proposition

For any complex number $\alpha \in \mathbb{C}$

$$R(M, \alpha x) = R(M, x).$$

Rayleigh Quotient (continued)

Proposition

For any Hermitian matrix $M \in M(n \times n; \mathbb{C})$ (i.e., $M^ = M$)*

$$R(M, x) \in \mathbb{R},$$

$$\lambda_{\min} \leq R(M, x) \leq \lambda_{\max},$$

where $\lambda_{\min}, \lambda_{\max} \in \mathbb{R}$ are the smallest and the greatest (real) eigenvalues of matrix M . Moreover, those bounds are attained by $R(M, x)$ by the corresponding eigenvectors $x \in \mathbb{C}^n$.

Rayleigh Quotient (continued)

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where $\lambda_{\min}, \lambda_{\max} \in \mathbb{R}$ are the smallest and the greatest (real) eigenvalues of matrix M . Moreover, those bounds are attained by $R(M, x)$ by the corresponding eigenvectors $x \in \mathbb{C}^n$.

Proof.

As $R(M, x)^* = R(M, x)$, it follows that $R(M, x) \in \mathbb{R}$. Let $v_1, \dots, v_n \in \mathbb{C}^n$ be a unitary orthonormal basis of \mathbb{C}^n , in which matrix of M is diagonal (i.e., it consist of eigenvectors v_i of matrix M such that $Mv_i = \lambda_i v_i$ and $v_j^T M v_i = 0$ for $i \neq j$). Let

$$x = \alpha_1 v_1 + \dots + \alpha_n v_n.$$

Rayleigh Quotient (continued)

Proof.

Then

$$R(M, x) = \frac{\sum_{i=1}^n \lambda_i |\alpha_i|^2}{\sum_{i=1}^n |\alpha_i|^2}.$$

Since $\lambda_{\min} \leq \lambda_i \leq \lambda_{\max}$, it follows that

$$\lambda_{\min} \leq \frac{\sum_{i=1}^n \lambda_i |\alpha_i|^2}{\sum_{i=1}^n |\alpha_i|^2} \leq \lambda_{\max}.$$

The bounds are attained for $x = v_i$ where $Mv_i = \lambda_{\min}v_i$ and for $x = v_j$ where $Mv_j = \lambda_{\max}v_j$. □

Rayleigh Quotient (continued)

Proposition

For any matrix $M \in M(n \times n; \mathbb{C})$ and any vector $x \in \mathbb{C}^n$ the Rayleigh quotient

$$\lambda = R(M, x) = \frac{x^* M x}{x^* x},$$

is the least square solution of the (possibly inconsistent) equation

$$Mx = \lambda x.$$

Rayleigh Quotient (continued)

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For any matrix $M \in M(n \times n; \mathbb{C})$ and any vector $x \in \mathbb{C}^n$ the Rayleigh quotient

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is the least square solution of the (possibly inconsistent) equation

$$Mx = \lambda x.$$

Proof.

The orthogonal projection of Mx onto $V = \text{lin}(x)$ is equal to

$$P_V(Mx) = \frac{x^*(Mx)}{x^* x} x.$$

Rayleigh Quotient (continued)

Proposition

For any fixed symmetric matrix $M = M^T \in M(n \times n; \mathbb{R})$ the eigenvectors of M are stationary points of the Rayleigh quotient, that is if $Mx = \lambda x$ for some $x \in \mathbb{R}^n, x \neq \mathbf{0}$ then

$$\nabla_x R(M, x) = \mathbf{0}.$$

Rayleigh Quotient (continued)

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$$\nabla_x R(M, x) = \mathbf{0}.$$

Proof.

$$\begin{aligned} \frac{\partial R}{\partial x_j}(M, x) &= \frac{\frac{\partial}{\partial x_j}(x^T M x)(x^T x) - (x^T M x) \frac{\partial}{\partial x_j}(x^T x)}{(x^T x)^2} = \\ &= \frac{2(Mx)_j(x^T x) - (x^T M x)2x_j}{(x^T x)^2} = \\ &= \frac{2}{x^T x} (Mx - R(M, x)x)_j, \end{aligned}$$

where $(Mx)_j$ denotes the j -th entry of the vector Mx .

Eigenvalue Decomposition

Proposition

Let $M \in M(n \times n; \mathbb{C})$ be a matrix such that there exists basis $\mathcal{A} = (v_1, \dots, v_n)$ of \mathbb{C}^n and numbers $\lambda_1, \dots, \lambda_n \in \mathbb{C}$ such that

$$M = CDC^*,$$

where $C = M(\text{id})_{\mathcal{A}}^{st}$ and $D = \text{diag}(\lambda_1, \dots, \lambda_n)$. Then

$$M = \sum_{i=1}^n \lambda_i v_i v_i^*,$$

where $v_i v_i^$ are rank 1 matrices.*

Eigenvalue Decomposition (continued)

Proof.

$$M = \sum_{i=1}^n C D_i C^* = \left(\sum_{i=1}^n \lambda_i C_i \right) C^* = \sum_{i=1}^n \lambda_i C_i C^*,$$

where $D_i = \text{diag}(0, \dots, 0, \lambda_i, 0, \dots, 0)$ and $C_i \in M(n \times n; \mathbb{C})$ is a zero matrix with i -th column replaced with eigenvector v_i . Then

$$C_i C^* = C_i C_i^* = v_i v_i^*.$$



Eigenvalue Decomposition (continued)

Corollary

Let $M \in M(n \times n; \mathbb{C})$ be a Hermitian matrix (i.e. $M^ = M$). Let $v_1, \dots, v_n \in \mathbb{C}^n$ be a unitary orthonormal basis consisting of eigenvectors of M corresponding to eigenvalues $\lambda_1, \dots, \lambda_n \in \mathbb{R}$. Then*

$$M = \sum_{i=1}^n \lambda_i v_i v_i^*.$$

Sherman–Morrison Formula

The following formula expresses the inverse of rank 1 update of matrix A .

Proposition

*For any matrix invertible $A \in M(n \times n; \mathbb{C})$ and vectors $v, w \in \mathbb{C}$ such that $1 + w^*Av \neq 0$ the matrix $A + vw^*$ is invertible and*

$$(A + vw^*)^{-1} = A^{-1} - \frac{A^{-1}vw^*A^{-1}}{1 + w^*A^{-1}v}.$$

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Proof.

First we show that

$$\begin{aligned}(I + uw^*)^{-1} &= I - \frac{uw^*}{1 + w^*u}. \\(I + uw^*) \left(I - \frac{uw^*}{1 + w^*u} \right) &= \\&= I - \frac{uw^*}{1 + w^*u} + uw^* - w^*u \frac{uw^*}{1 + w^*u} = I.\end{aligned}$$

Sherman–Morrison Formula (continued)

Proof.

Since A is invertible there exists $u \in \mathbb{C}^n$ such that $v = Au$, i.e. $u = A^{-1}v$. Then

$$A + vw^* = A(I + uw^*),$$

and the matrix $A + vw^*$ is invertible if and only if the matrix $I + uw^*$ is invertible. Moreover

$$\begin{aligned}(A + vw^*)^{-1} &= (I + uw^*)^{-1}A^{-1} = \left(I - \frac{uw^*}{1 + w^*u}\right)A^{-1} = \\ &= A^{-1} - \frac{A^{-1}vw^*A^{-1}}{1 + w^*A^{-1}v}.\end{aligned}$$



Singular Value Decomposition – SVD

Theorem

For any matrix $A \in M(m \times n; \mathbb{C})$ there exist unitary matrices $U \in M(m \times m; \mathbb{C})$, $V \in M(n \times n; \mathbb{C})$ and a unique (real) generalized diagonal matrix

$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in M(m \times n; \mathbb{R})$ such that

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0,$$

where $r = r(A)$ oraz

$$A = U\Sigma V^*.$$

Singular Value Decomposition – SVD

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$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0,$$

where $r = r(A)$ oraz

$$A = U\Sigma V^*.$$

Remark

Matrices U, V are not uniquely determined (unlike the matrix Σ).

Singular Value Decomposition – SVD (continued)

Proof.

Let $\sigma_1 = \|A\|_2$. By the definition of $\|\cdot\|_2$ and the compactness of a ball in \mathbb{C}^m there exist vectors $v_1 \in \mathbb{C}^m$ and vectors $u_1 \in \mathbb{C}^n$ such that $\|v_1\|_2 = \|u_1\|_2 = 1$, and

$$Av_1 = \sigma_1 u_1.$$

Let $V_1 \in M(n \times n; \mathbb{C})$ be a unitary matrix with the first column equal to vector v_1 , and let $U_1 \in M(m \times m; \mathbb{C})$ be a unitary matrix with first column equal to u_1 . Then

$$U_1^* A V_1 = \begin{bmatrix} \sigma_1 & w^* \\ \mathbf{0} & B \end{bmatrix},$$

where $w \in \mathbb{C}^{n-1}$ and $B \in M((m-1) \times (n-1); \mathbb{C})$. □

⁰see L. N. Trefethen, D. Bau, III, *Numerical Linear Algebra*, SIAM 

Singular Value Decomposition – SVD (continued)

Proof.

Then

$$\left\| \begin{bmatrix} \sigma_1 & w^* \\ \mathbf{0} & B \end{bmatrix} \begin{bmatrix} \sigma_1 \\ w \end{bmatrix} \right\|_2 \geq \sigma_1^2 + w^* w = \sqrt{\sigma_1^2 + w^* w} \left\| \begin{bmatrix} \sigma_1 \\ w \end{bmatrix} \right\|_2.$$

It follows that $w = \mathbf{0}$, otherwise σ_1 is not maximal. By the inductive assumption there exists unitary matrices $V_2 \in M((n-1) \times (n-1); \mathbb{C})$ and $U_2 \in M((m-1) \times (m-1); \mathbb{C})$ such that

$$A = U_1 \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & U_2 \end{bmatrix} \begin{bmatrix} \sigma_1 & \mathbf{0} \\ \mathbf{0} & \Sigma_2 \end{bmatrix} \begin{bmatrix} 1 & \mathbf{0} \\ \mathbf{0} & V_2 \end{bmatrix}^* V_1^*.$$



Singular Value Decomposition – SVD (continued)

Proof.

To prove uniqueness of Σ , assume there exists a vector w corresponding to the singular value σ_1 , such that v_1, w are linearly independent (i.e., $\|Aw\|_2 = \sigma_1$) such that $\|w\|_2 = 1$ (otherwise the subspace $\text{lin}(v_1)^\perp$ is uniquely determined). Then the vector

$$v_2 = \frac{w - (v_1^* w) v_1}{\|w - (v_1^* w) v_1\|_2},$$

equal to the unit vector of the projection of vector w onto the subspace $\text{lin}(v_1)^\perp \subset \mathbb{C}^m$, satisfies the condition

$$w = \alpha v_1 + \beta v_2,$$

where $|\alpha|^2 + |\beta|^2 = 1$ (vector w is a unit vector and vectors v_1, v_2 are orthogonal). □

Singular Value Decomposition – SVD (continued)

Proof.

Then $\|Av\|_2 \leq \sigma_1$, and if $\|Av\|_2 < \sigma_1$, then

$$\|Aw\|_2^2 = |\alpha|^2 \|Av_1\|_2^2 + |\beta|^2 \|Av_2\|_2^2 < \sigma_1,$$

which leads to contradiction. Therefore, vector w is a vector corresponding to the singular value σ_1 of matrix B . The claim follow by induction. □

Real Singular Value Decomposition

Theorem

For any matrix $A \in M(m \times n; \mathbb{R})$ there exists orthogonal matrices $U \in M(m \times m; \mathbb{R})$, $V \in M(n \times n; \mathbb{C})$ and a uniquely determined generalized diagonal matrix

$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in M(m \times n; \mathbb{R})$ such that

$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0,$$

where $r = r(A)$ and

$$A = U\Sigma V^T.$$

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$$\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0,$$

where $r = r(A)$ and

$$A = U\Sigma V^T.$$

Remark

As before, the orthogonal matrices U, V are not uniquely determined.

Real Singular Value Decomposition (continued)

The following proof, using the spectral theorem, after a slight modification works in the complex case too.

Proof.

Matrix $A^T A \in M(n \times n; \mathbb{R})$ is symmetric and positive semidefinite hence there exists orthonormal basis (not uniquely determined) $v_1, \dots, v_n \in \mathbb{R}^n$ of \mathbb{R}^n consisting of eigenvectors of $A^T A$ such that

$$v_i^T A^T A v_j = \begin{cases} 0 & i \neq j, \\ \lambda_i & i = j, \end{cases}, \quad \text{for } i, j = 1, \dots, r,$$

$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_r > 0,$$

$$\lambda_{r+1} = \dots \lambda_n = 0,$$

where $\lambda_i \geq 0$ is an eigenvalue of $A^T A$ corresponding to eigenvector $v_i \in \mathbb{R}^n$ and $r \in \mathbb{N}$ is some natural number such that $1 \leq r \leq n$.

Real Singular Value Decomposition (continued)

Proof.

Let

$$\sigma_i = \sqrt{\lambda_i}, \quad \text{for } i = 1, \dots, n,$$

and

$$u_i = \frac{1}{\sigma_i} A v_i \in \mathbb{R}^m, \quad \text{for } i = 1, \dots, r.$$

Then

$$u_i^\top u_j = \frac{1}{\sigma_i \sigma_j} v_i^\top A^\top A v_j = \begin{cases} 0 & i \neq j, \\ 1 & i = j, \end{cases}, \quad \text{for } i, j = 1, \dots, r.$$

Moreover

$$A v_i = \mathbf{0}, \quad \text{for } i = r + 1, \dots, n,$$

$$\text{as } \|A v_i\|^2 = v_i^\top A^\top A v_i = 0.$$

Real Singular Value Decomposition (continued)

Proof.

Let $u_1, \dots, u_r, u_{r+1}, \dots, u_m \in \mathbb{R}^m$ be an extension of some orthonormal basis of $\text{im}A \subset \mathbb{R}^m$ to some orthonormal basis \mathbb{R}^m (both not uniquely determined). Let $U \in M(m \times m; \mathbb{R})$ be an orthogonal matrix which columns are equal to $u_1, \dots, u_m \in \mathbb{R}^m$, respectively and let $V \in M(n \times n; \mathbb{R})$ be an orthogonal matrix which columns are equal to $v_1, \dots, v_n \in \mathbb{R}^n$, respectively. Let

$$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in M(m \times n; \mathbb{R}).$$

Real Singular Value Decomposition (continued)

Proof.

Then

$$U\Sigma V^T v_i = U\Sigma_i e_i = \sigma_i u_i = \sigma_i \left(\frac{1}{\sigma_i} A v_i \right) = A v_i,$$

for $i = 1, \dots, r$, and

$$U\Sigma V^T v_i = U\Sigma_i e_i = 0 u_i = \mathbf{0},$$

for $i = r + 1, \dots, n$. Therefore

$$A = U\Sigma V^T,$$

and $r(A) = r$ as $r(\Sigma) = r$ and matrices U, V are non-singular. For the uniqueness of matrix Σ proceed like in the complex case. \square

Real Singular Value Decomposition (continued)

Remark

The proof implies that

$$A = \sum_{i=1}^r \sigma_i u_i v_i^{\mathsf{T}}.$$

Real Singular Value Decomposition (continued)

Remark

The proof implies that

$$A = \sum_{i=1}^r \sigma_i u_i v_i^T.$$

Remark

The preceding proof works after small modification in the complex case.

Pseudoinverse

Definition

With the same notation

$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in M(m \times n; \mathbb{R})$ set

$$\Sigma^+ = \text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \in M(n \times m; \mathbb{R}),$$

$$A^+ = V\Sigma^+U^*.$$

Matrix A^+ is called **pseudoinverse** or **Moore–Penrose pseudoinverse** of A (note that matrix Σ^+ is of the same size as Σ^T).

Pseudoinverse (continued)

Proposition

For any matrix $A \in M(m \times n; \mathbb{C})$ there exists at most one matrix $A^+ \in M(n \times m; \mathbb{C})$ such that

i) $AA^+A = A,$

Pseudoinverse (continued)

Proposition

For any matrix $A \in M(m \times n; \mathbb{C})$ there exists at most one matrix $A^+ \in M(n \times m; \mathbb{C})$ such that

- i) $AA^+A = A$,
- ii) $A^+AA^+ = A^+$,

Pseudoinverse (continued)

Proposition

For any matrix $A \in M(m \times n; \mathbb{C})$ there exists at most one matrix $A^+ \in M(n \times m; \mathbb{C})$ such that

- i) $AA^+A = A$,
- ii) $A^+AA^+ = A^+$,
- iii) $(AA^+)^* = AA^+$,

Pseudoinverse (continued)

Proposition

For any matrix $A \in M(m \times n; \mathbb{C})$ there exists at most one matrix $A^+ \in M(n \times m; \mathbb{C})$ such that

- i) $AA^+A = A$,
- ii) $A^+AA^+ = A^+$,
- iii) $(AA^+)^* = AA^+$,
- iv) $(A^+A)^* = A^+A$,

Pseudoinverse (continued)

Proposition

For any matrix $A \in M(m \times n; \mathbb{C})$ there exists at most one matrix $A^+ \in M(n \times m; \mathbb{C})$ such that

- i) $AA^+A = A$,
- ii) $A^+AA^+ = A^+$,
- iii) $(AA^+)^* = AA^+$,
- iv) $(A^+A)^* = A^+A$,

(in particular matrices AA^+ , A^+A are Hermitian). Moreover, matrix

$$A^+ = V\Sigma^+U^*,$$

satisfies the above conditions.

Pseudoinverse (continued)

Proof.

Let

$$A = U\Sigma V^*,$$

$$A^+ = V\Sigma^+ U^*,$$

be the singular value decomposition of A , where

$$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in M(m \times n; \mathbb{R}),$$

$$\Sigma^+ = \text{diag}(\sigma_1^{-1}, \dots, \sigma_r^{-1}, 0, \dots, 0) \in M(n \times m; \mathbb{R}).$$

Then

$$\Sigma\Sigma^+ = \left[\begin{array}{c|c} I_r & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array} \right] \in M(m \times m; \mathbb{R}), \quad \Sigma^+\Sigma = \left[\begin{array}{c|c} I_r & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{0} \end{array} \right] \in M(n \times n; \mathbb{R}).$$

In particular

$$\Sigma\Sigma^+\Sigma = \Sigma, \quad \Sigma^+\Sigma\Sigma^+ = \Sigma^+.$$

Pseudoinverse (continued)

Proof.

Then

i)

$$AA^+A = (U\Sigma V^*)V\Sigma^+U^*(U\Sigma V^*) = U(\Sigma\Sigma^+\Sigma)V^* = A,$$

Pseudoinverse (continued)

Proof.

Then

i)

$$AA^+A = (U\Sigma V^*)V\Sigma^+U^*(U\Sigma V^*) = U(\Sigma\Sigma^+\Sigma)V^* = A,$$

ii)

$$A^+AA^+ = (V\Sigma^+U^*)U\Sigma V^*(V\Sigma^+U^*) = V(\Sigma^+\Sigma\Sigma^+)U^* = A^+,$$

Pseudoinverse (continued)

Proof.

Then

i)

$$AA^+A = (U\Sigma V^*)V\Sigma^+U^*(U\Sigma V^*) = U(\Sigma\Sigma^+\Sigma)V^* = A,$$

ii)

$$A^+AA^+ = (V\Sigma^+U^*)U\Sigma V^*(V\Sigma^+U^*) = V(\Sigma^+\Sigma\Sigma^+)U^* = A^+,$$

iii)

$$\begin{aligned}(A^+A)^* &= A^*(A^+)^* = (U\Sigma V^*)^*(V\Sigma^+U^*)^* = \\&= (V\Sigma^*U^*)(U(\Sigma^+)^*V^*) = V(\Sigma^+\Sigma)^*V^* = V(\Sigma^+\Sigma)V^* = \\&= (V\Sigma^+U^*)(U\Sigma V^*) = V(\Sigma^+\Sigma)V^* = A^+A.\end{aligned}$$

Pseudoinverse (continued)

Proof.

Then

i)

$$AA^+A = (U\Sigma V^*)V\Sigma^+U^*(U\Sigma V^*) = U(\Sigma\Sigma^+\Sigma)V^* = A,$$

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iv) j.w.

Pseudoinverse (continued)

Proof.

Assume that matrices A^+, A'^+ satisfy conditions i) – iv). Then

$$\begin{aligned} A^+ &= A^+ A A^+ = A^+ (A) A^+ = A^+ (A A'^+ A) A^+ = A^+ ((A) A'^+ (A)) A^+ = \\ &= A^+ ((A A'^+ A) A'^+ (A A'^+ A)) A^+ = (A^+ A)^* (A'^+ A)^* A'^+ (A A'^+)^* (A A^+)^* = \\ &= (A^* (A^+)^*) (A^* (A'^+)^*) A'^+ ((A'^+)^* A^*) ((A^+)^* A^*) = \\ &= (A^* (A^+)^* A^*) (A'^+)^* A'^+ (A'^+)^* (A^* (A^+)^* A^*) = \\ &= (A (A^+)^* A)^* (A'^+)^* A'^+ (A'^+)^* (A (A^+)^* A)^* = \\ &= A^* (A'^+)^* A'^+ (A'^+)^* A^* = \end{aligned}$$

Pseudoinverse (continued)

Proof.

$$\begin{aligned} &= A^*(A'^+)^*A'^+(A'^+)^*A^* = \\ &= (A'^+A)^*A'^+(AA'^+)^* = (A'^+A)A'^+(AA'^+) = \\ &= A'^+(AA'^+A)A'^+ = A'^+AA'^+ = A'^+. \end{aligned}$$

Singular Value Decomposition – Remarks

Remarks

- i) *if matrix A is real then there exists real orthogonal matrices U, V such that $A = U\Sigma V^T$,*
- ii) *when $\sigma_1 > \sigma_2 > \dots > \sigma_r > 0$, that is the singular values are pairwise different then the columns $1, 2, \dots, r$ of U i V are uniquely determined up to a constant $\alpha_i \in \mathbb{C}$ (respectively $\alpha_i \in \mathbb{R}$, when A is real) such that $|\alpha_i| = 1$,*
- iii) *when $A \in M(n \times n; \mathbb{C})$ and $\det A \neq 0$ then $A^+ = A^{-1}$,*
- iv) *the following matrix norms of A are determined by the singular values of A , i.e.,*

$$\|A\|_F = \sqrt{\sum_{i=1}^r \sigma_i^2},$$

$$\|A\|_2 = \sigma_1,$$

Singular Value Decomposition – Remarks (continued)

Remarks

i) let $A = U\Sigma V^*$, that is

$$AV = U\Sigma.$$

Denote by u_1, \dots, u_m the columns of matrix $U \in M(m \times m; \mathbb{R})$ and by v_1, \dots, v_n the columns of matrix $V \in M(n \times n; \mathbb{R})$. Then for $i = 1, \dots, \max m, n$

$$Av_i = \sigma_i u_i.$$

Moreover

$$\ker A = \text{lin}(v_{r+1}, \dots, v_n)$$

$$\text{im} A = \text{lin}(u_1, \dots, u_r).$$

Singular Value Decomposition – Remarks (continued)

Remarks

- vi) for any $k \leq r$ let $\Sigma_k = \text{diag}(\sigma_1, \dots, \sigma_k, 0, \dots, 0) \in M(m \times n; \mathbb{R})$.
Then the matrix

$$A_k = U \Sigma_k V^*,$$

satisfies the condition: for any matrix $B \in M(m \times n; \mathbb{C})$ of rank k

$$\|A - B\|_2 \geq \|A - A_k\|_2 = \sigma_{k+1},$$

$$\|A - B\|_F \geq \|A - A_k\|_F = \sqrt{\sigma_{k+1}^2 + \dots + \sigma_r^2},$$

where, assuming $A = [a_{ij}] \in M(m \times n; \mathbb{C})$ the norms are defined as follows

$$\|A\|_F = \sqrt{\text{Tr}(A^* A)} = \sqrt{\text{Tr}(A A^*)} = \sqrt{\sum_{i=1, \dots, n} \sum_{j=1, \dots, m} |a_{ij}|^2},$$

$$\|A\|_2 = \sup\{\|Ax\|_2 \in \mathbb{R} \mid x \in \mathbb{R}^n, \|x\|_2 = 1\} = \sqrt{\lambda_{\max}(A^* A)},$$

$$\|x\|_2 = \sqrt{x^* x}.$$

The Best Low Rank Approximation

Proposition

Let $A \in M(m \times n; \mathbb{C})$ be any matrix and let $A = U\Sigma V^*$ be its singular value decomposition, where

$$\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in M(m \times n; \mathbb{R}),$$

and $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$, i.e., $r(A) = r$. Then, for any k such that $0 \leq k < r$ and for any matrix $B \in M(m \times n; \mathbb{C})$ such that $r(B) = k$ it holds

$$\|A - A_k\| \leq \|A - B\|,$$

where

$$A_k = U\Sigma_k V^*,$$

$$\Sigma_k = \text{diag}(\sigma_1, \dots, \sigma_k, 0, \dots, 0) \in M(m \times n; \mathbb{R}),$$

that is, matrix A_k of rank k is the best approximation of matrix A among matrices of rank k of the same size as matrix A (in the norm

$$\|A\| = \sup_{\|x\|_2=1} \|Ax\|_2).$$

The Best Low Rank Approximation (continued)

Proof.

Obviously $r(A_k) = k$. Moreover

$$\begin{aligned}\|A - A_k\| &= \|U \operatorname{diag}(0, \dots, \sigma_{k+1}, \dots, \sigma_r, 0 \dots, 0) V^*\| = \\ &= \|\operatorname{diag}(0, \dots, \sigma_{k+1}, \dots, \sigma_r, 0 \dots, 0)\| = \sigma_{k+1}.\end{aligned}$$

Let $B \in M(m \times n; \mathbb{C})$ be any matrix such that $r(B) = k$. Let

$$W = \{w \in \mathbb{R}^m \mid Bw = \mathbf{0}\}.$$

Let $w_1, \dots, w_{n-k} \in \mathbb{C}^n$ be an unitary orthonormal basis of subspace $W \subset \mathbb{C}^n$. Let $v_1, \dots, v_n \in \mathbb{C}^n$ denote columns of matrix V . Let

$$v \in \operatorname{lin}(v_1, \dots, v_{k+1}) \cap W \neq \{\mathbf{0}\},$$

be any (non-zero) vector such that

$$\|v\| = 1.$$

The Best Low Rank Approximation (continued)

Proof.

Then

$$\begin{aligned}\|A - B\| &\geq \|(A - B)v\| = \|Av\| = \\&= \left\| \sum_{i=1}^r (u_i \sigma_i v_i^*) v \right\| = \left\| \sum_{i=k+1}^r ((v_i^* v) u_i \sigma_i) \right\| = \\&= \sum_{i=k+1}^r \sigma_i^2 (v_i^* v)^2 \geq \sigma_{k+1} \sum_{i=k+1}^r (v_i^* v)^2 \geq \sigma_{k+1},\end{aligned}$$

since

$$\|Vv\|^2 = \sum_{i=1}^n (v_i^* v)^2 = 1 \geq \sum_{i=k+1}^r (v_i^* v)^2.$$



Singular Value Decomposition – Example

Let

$$A = \begin{bmatrix} 5 & 5 \\ -1 & 7 \end{bmatrix}.$$

Then, assuming $A = U\Sigma V^*$, we have

$$\begin{aligned} A^*A &= (V\Sigma^*U^*)(U\Sigma V^*) = V\Sigma^*\Sigma V^* = \begin{bmatrix} 26 & 18 \\ 18 & 74 \end{bmatrix} = \\ &= \begin{bmatrix} \frac{1}{\sqrt{10}} & \frac{3}{\sqrt{10}} \\ \frac{3}{\sqrt{10}} & -\frac{1}{\sqrt{10}} \end{bmatrix} \begin{bmatrix} 80 & 0 \\ 0 & 20 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{10}} & \frac{3}{\sqrt{10}} \\ \frac{3}{\sqrt{10}} & -\frac{1}{\sqrt{10}} \end{bmatrix}, \\ AA^* &= (U\Sigma V^*)(V\Sigma^*U^*) = U\Sigma\Sigma^*U^* = \begin{bmatrix} 50 & 30 \\ 30 & 50 \end{bmatrix} = \\ &= \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 80 & 0 \\ 0 & 20 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}. \end{aligned}$$

Singular Value Decomposition – Example (continued)

Hence

$$A = \begin{bmatrix} 5 & 5 \\ -1 & 7 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 4\sqrt{5} & 0 \\ 0 & 2\sqrt{5} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{10}} & \frac{3}{\sqrt{10}} \\ \frac{3}{\sqrt{10}} & -\frac{1}{\sqrt{10}} \end{bmatrix},$$

that is

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}, \quad \Sigma = \begin{bmatrix} 4\sqrt{5} & 0 \\ 0 & 2\sqrt{5} \end{bmatrix}, \quad V = \begin{bmatrix} \frac{1}{\sqrt{10}} & \frac{3}{\sqrt{10}} \\ \frac{3}{\sqrt{10}} & -\frac{1}{\sqrt{10}} \end{bmatrix},$$

$$A = U\Sigma V^*,$$

therefore the best rank 1 approximation of matrix A in the norm $\|\cdot\|_2$ oraz $\|\cdot\|_F$ is

$$A_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 4\sqrt{5} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{10}} & \frac{3}{\sqrt{10}} \\ \frac{3}{\sqrt{10}} & -\frac{1}{\sqrt{10}} \end{bmatrix} = \begin{bmatrix} 2 & 6 \\ 2 & 6 \end{bmatrix}.$$

Singular Value Decomposition – Example (continued)

$$A = \begin{bmatrix} 5 & 5 \\ -1 & 7 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 4\sqrt{5} & 0 \\ 0 & 2\sqrt{5} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{10}} & \frac{3}{\sqrt{10}} \\ \frac{3}{\sqrt{10}} & -\frac{1}{\sqrt{10}} \end{bmatrix},$$

$$A_1 = \begin{bmatrix} 2 & 6 \\ 2 & 6 \end{bmatrix},$$

$$B = A - A_1 = \begin{bmatrix} 3 & -1 \\ -3 & 1 \end{bmatrix},$$

and

$$\|B\|_F = \sqrt{3^2 + (-1)^2 + 3^2 + (-1)^2} = 2\sqrt{5} = \sigma_2(A),$$

$$\det(B^*B - \lambda I) = \det \begin{bmatrix} 18 - \lambda & -6 \\ -6 & 2 - \lambda \end{bmatrix} = \lambda(\lambda^2 - 20),$$

hence

$$\|B\|_2 = \sqrt{\lambda_{\max}(B^*B)} = \sqrt{20} = 4\sqrt{5}.$$

Optimal Solution of a System of Linear Equations

Definition

For any system of linear equations $Ax = b$ where $A \in M(m \times n; \mathbb{C})$, $b \in M(m \times 1; \mathbb{C})$ the vector $x \in \mathbb{C}^n$ is called the optimal solution if

$$\|Ax - b\|_2 \leq \|Ay - b\|_2 \text{ for any } y \in \mathbb{C}^n,$$

and if $\|Ax - b\|_2 = \|Ax' - b\|_2$ then $\|x\|_2 \leq \|x'\|_2$,

Proposition

For any matrices $A \in M(m \times n; \mathbb{C})$, $b \in M(m \times 1; \mathbb{C})$ the vector

$$x = A^+ b$$

is the optimal solution of the system $Ax = b$.

Optimal Solution of a System of Linear Equations

Proof.

Let $P = AA^+$ be the matrix of orthogonal projection onto $\text{im}(A)$.
Then for any x

$$\begin{aligned}\|Ax - b\|_2 &= \|Ax - Pb + (P - I)b\|_2 = \\ &= \|Ax - Pb\|_2 + \|(P - I)b\|_2 \geq \|(P - I)b\|_2.\end{aligned}$$

The lower bound (which does not depend on x) is attained when $x = A^+b$. Assume that $Ax = Ax'$ where $x = A^+b \in \text{im}(A^*)$.
Therefore there exists $n \in \ker A$ such that $x' = x + n$ where x and n are perpendicular. Therefore

$$\|x'\|_2 = \|x\|_2 + \|n\|_2 \geq \|x\|_2.$$



Example

For

$$A = \begin{bmatrix} 1 & 1 \\ 2 & 3 \\ 1 & 1 \end{bmatrix}, \quad B = \begin{bmatrix} 3 \\ 0 \\ -1 \end{bmatrix}.$$

$$A^+ = \begin{bmatrix} \frac{3}{2} & -1 & \frac{3}{2} \\ -1 & 1 & -1 \end{bmatrix}$$

It follows

$$A^+A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad A^+B = \begin{bmatrix} 3 \\ -2 \end{bmatrix},$$

which is the optimal solution of $AX = B$.

Hadamard's inequality

Proposition

For any matrix $A \in M(n \times n; \mathbb{R})$

$$|\det A| \leq \|c_1\| \cdot \dots \cdot \|c_n\|,$$

where c_i is the i -th column of matrix A and

$$\|c_i\| = \sqrt{c_i^T c_i},$$

is the (Euclidean) length of the i -th column, for $i = 1, \dots, n$.

Moreover, the equality holds if and only if

$$c_i \perp c_j, \quad \text{for } i \neq j.$$

Hadamard's inequality (continued)

Proof.

If $c_i = \mathbf{0}$ or $\det A = 0$ then there is nothing to prove. Dividing each column of matrix A by its length the problem reduces to the following one

$$|\det A| \leq 1,$$

where $\|c_i\| = 1$ for $i = 1, \dots, n$. Let

$$M = A^T A.$$

Then matrix M is a positive definite symmetric matrix. Moreover,

$$\operatorname{Tr} M = \sum_{i=1}^n m_{ii} = n,$$

where $M = [m_{ij}]$ as columns of matrix A are of length 1.

Hadamard's inequality (continued)

Proof.

By spectral theorem matrix M is diagonalizable and therefore

$$\det M = \lambda_1 \cdot \dots \cdot \lambda_n.$$

Moreover

$$\det M = \det(A^T A) = (\det A)^2 = \lambda_1 \cdot \dots \cdot \lambda_n \leq \left(\frac{\lambda_1 + \dots + \lambda_n}{n} \right)^n = 1,$$

by the Arithmetic-Geometric Mean Inequality. The upper bound is achieved when

$$\lambda_1 = \lambda_2 = \dots = \lambda_n = 1,$$

i.e., when $M = A^T A = I$ that is when columns of A are pairwise perpendicular.



Cauchy–Schwarz Inequality

Proposition

Let $A \in M(n \times n; \mathbb{R})$ be a positive semidefinite symmetric matrix.
Then for any $x, y \in \mathbb{R}^n$

$$|x^T A y| \leq (x^T A x)^{\frac{1}{2}} (y^T A y)^{\frac{1}{2}}.$$

Proof.

For any $t \in \mathbb{R}$,

$$0 \leq (x - ty)^T A (x - ty) = (y^T A y) t^2 - 2 (x^T A y) t + (x^T A x).$$

Hence, the discriminant

$$\Delta = 4 (x^T A y)^2 - 4 (x^T A x) (y^T A y) \leq 0.$$



Cauchy–Schwarz Inequality (continued)

Definition

Vector $x \in \mathbb{R}^n$ is **isotropic** (with respect to a symmetric matrix A) if $x^T A x = 0$.

Corollary

Let $A \in M(n \times n; \mathbb{R})$ be a symmetric positive semidefinite matrix. Then $x \in \mathbb{R}^n$ is isotropic if and only if $Ax = \mathbf{0}$.

Proof.

Assume $y \in \mathbb{R}^n$ is isotropic in the proof of Cauchy–Schwarz inequality. Then the linear function

$$-2(x^T A y) t + (x^T A x) \geq 0,$$

is non-negative for any $x \in \mathbb{R}^n$. This implies $x^T A y = 0$ for any $x \in \mathbb{R}^n$, i.e. $Ay = \mathbf{0}$. □

Convex Cone

Definition

A subset $C \subset \mathbb{R}^n$ is a **cone**, if

i) for any $v, w \in C$

$$v + w \in C,$$

ii) for any $v \in C$ and any $\alpha \in \mathbb{R}$ such that $\alpha \geq 0$,

$$\alpha v \in C.$$

The cone C is **pointed** if it does not contain a one-dimensional subspace of \mathbb{R}^n (i.e, a line). The cone C is **(closed) polyhedral** if it equal to the intersection of finite (closed) half-spaces in \mathbb{R}^n .

Dual Cone

Definition

Let $A \subset \mathbb{R}^n$ be any subset. Let $v \cdot w$ be a scalar product in \mathbb{R}^n . Then the set

$$A^\vee = \{v \in \mathbb{R}^n \mid v \cdot w \geq 0 \text{ for any } w \in A\},$$

is called the dual cone of the set A .

Proposition

For any subset $A \subset \mathbb{R}^n$ the set A^\vee is a closed convex cone.

Proof.

Exercise. □

Cone Spanned by Set

Definition

A cone $C \subset \mathbb{R}^n$ is spanned by set $A \subset \mathbb{R}^n$ if

$$C = \{\alpha_1 v_1 + \dots + \alpha_k v_k \in \mathbb{R}^n \mid v_1, \dots, v_k \in A, \alpha_1, \dots, \alpha_k \geq 0, k \geq 1\}.$$

We write

$$C = \text{cone}(A),$$

and if $A = \{v_1, \dots, v_k\}$

$$C = \text{cone}(v_1, \dots, v_k).$$

Extremal Rays of a Cone

Definition

Let $C \subset \mathbb{R}^n$ be a (convex) cone. Vector (or a half-line spanned by it) $v \in C, v \neq \mathbf{0}$ is an **extremal ray** of cone C , if for any $v_1, v_2 \in C$, if $v = v_1 + v_2$ then $v_1 = tv$ or $v_2 = tv$ for some $t \geq 0$.

The Positive Semidefinite Cone

Definition

Let

$$\mathbb{S}^n = \{A \in M(n \times n; \mathbb{R}) \mid A^T = A\} \subset M(n \times n; \mathbb{R}),$$

be the $\binom{n+1}{2}$ subspace of symmetric matrices with the (standard) scalar product given by

$$A \cdot B = \text{Tr}(AB),$$

for any $A, B \in \mathbb{S}^n$.

Definition

Let

$$C_{\geq 0} = \{A \in \mathbb{S}^n \mid A \text{ is positive semidefinite}\},$$

$$C_{> 0} = \{A \in \mathbb{S}^n \mid A \text{ is positive definite}\},$$

denote the **positive semidefinite** and **positive definite** cones, respectively.

The Positive Semidefinite Cone (continued)

Proposition

- i) *the positive semidefinite cone $C_{\geq 0}$ is a closed convex pointed cone,*
- ii) *the positive semidefinite cone $C_{\geq 0}$ is self-dual, i.e.*

$$C_{\geq 0}^{\vee} = C_{\geq 0},$$

with respect to the scalar product given by the trace,

- iii) *the positive semidefinite cone $C_{\geq 0}$ is spanned by rank 1 matrices vv^T , i.e.,*

$$C_{\geq 0} = \text{cone}(\{vv^T \in \mathbb{S}^n \mid v \in \mathbb{R}^n\}),$$

- iv) *the matrices vv^T are exactly the extremal rays of the cone $C_{\geq 0}$,*
- v)

$$\text{int } C_{\geq 0} = C_{> 0}.$$

The Positive Semidefinite Cone (continued)

Proposition

- i) *the positive semidefinite cone $C_{\geq 0}$ is a closed convex pointed cone,*
- ii) *the positive semidefinite cone $C_{\geq 0}$ is self-dual, i.e.*

$$C_{\geq 0}^{\vee} = C_{\geq 0},$$

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- iii) *the positive semidefinite cone $C_{\geq 0}$ is spanned by rank 1 matrices vv^T , i.e.,*

$$C_{\geq 0} = \text{cone}(\{vv^T \in \mathbb{S}^n \mid v \in \mathbb{R}^n\}),$$

- iv) *the matrices vv^T are exactly the extremal rays of the cone $C_{\geq 0}$,*
- v)

$$\text{int } C_{\geq 0} = C_{> 0}.$$

Proof.

Omitted. Involves mostly eigenvalue decomposition.



The Positive Semidefinite Cone (continued)

Remark

The positive semidefinite cone is described by polynomial inequalities given by the all principal minors (Sylvester's criterion). For example matrix

$$A = \begin{bmatrix} a & b \\ b & c \end{bmatrix},$$

is positive semidefinite if and only if

$$\begin{cases} a \geq 0, \\ c \geq 0, \\ ac - b^2 \geq 0. \end{cases}$$

The extremal rays of the positive semidefinite cone are exactly of the form

$$\begin{bmatrix} s \\ t \end{bmatrix} \begin{bmatrix} s & t \end{bmatrix} = \begin{bmatrix} s^2 & st \\ st & t^2 \end{bmatrix},$$

for any $s, t \in \mathbb{R}$.

The Positive Semidefinite Cone (continued)

Remark

When $\|v\| = 1$ the matrix vv^T is the matrix of the orthogonal (linear) projections onto $\text{lin}(v)$, i.e.

$$M(P_{\text{lin}(v)})_{st}^{st} = vv^T.$$

In general, for any $v \neq \mathbf{0}$

$$M(P_{\text{lin}(v)})_{st}^{st} = \frac{vv^T}{v^T v}.$$

Non-negative Polynomials

Definitions

Let $d \geq 1$. A polynomial $p(x)$ of degree $2d$ is **non-negative** if for any $x \in \mathbb{R}$

$$p(x) \geq 0.$$

Proposition

A polynomial $p(x)$ of degree $2d$ is non-negative if and only if all its real roots are of even multiplicity and if $a_{2d} > 0$ where $p(x) = a_{2d}x^{2d} + \dots$ (that is the leading coefficient is positive).

Proof.

Exercise.



Non-negative Polynomials (continued)

Proposition

A polynomial $p(x) = \sum_{i=0}^{2d} a_i x^i$ of degree $2d$ is non-negative if and only if there exists a symmetric positive semidefinite matrix

$M = [m_{ij}] \in M((d+1) \times (d+1); \mathbb{R})$ such that

$$a_k = \sum_{i+j=k} m_{ij},$$

for any $k = 0, \dots, 2d$ where rows and columns of matrix M are numbered from 0 to d . Moreover the correspondence is one-to-one.

Non-negative Polynomials (continued)

Proof.

(\Leftarrow) Let $\mathbf{x} = (1, x, x^2, \dots, x^d)$. Then

$$p(x) = \mathbf{x}^T M \mathbf{x} \geq 0.$$

(\Rightarrow)

$$p(z) = a_{2d} \prod_{i=1}^d (z - z_i)(z - \overline{z_i}),$$

where $z_i, \overline{z_i} \in \mathbb{C}$ are complex roots of $p(x)$. Let

$$q(x) = \sqrt{a_{2d}} \prod_{i=1}^d (x - z_i) = \sum_{i=0}^d c_i x^i.$$

Let

$$q_1(x) = \operatorname{Re} q(x) = \sum_{i=0}^d (\operatorname{Re} c_i) x^i,$$

$$q_2(x) = \operatorname{Im} q(x) = \sum_{i=0}^d (\operatorname{Im} c_i) x^i,$$

Non-negative Polynomials (continued)

Proof.

i.e.

$$q(x) = q_1(x) + \sqrt{-1}q_2.$$

Then for any $x \in \mathbb{R}$

$$\begin{aligned} p(x) &= q(x)\overline{q(x)} = |q(x)|^2 = q_1^2(x) + q_2^2(x) = \\ &= (v^T x)^2 + (w^T x)^2 = x^T (vv^T + ww^T)x, \end{aligned}$$

where

$$v = (\operatorname{Re} c_0, \operatorname{Re} c_1, \dots, \operatorname{Re} c_d) \in \mathbb{R}^{d+1},$$

$$w = (\operatorname{Im} c_0, \operatorname{Im} c_1, \dots, \operatorname{Im} c_d) \in \mathbb{R}^{d+1}.$$



Example

Let

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 2 & -1 \end{bmatrix}.$$

Then

$$M = A^T A = \begin{bmatrix} 2 & -2 & 1 \\ -2 & 5 & -2 \\ 1 & -2 & 2 \end{bmatrix},$$

is positive definite. Therefore, the polynomial

$$p(x) = \begin{bmatrix} 1 & x & x^2 \end{bmatrix} \begin{bmatrix} 2 & -2 & 1 \\ -2 & 5 & -2 \\ 1 & -2 & 2 \end{bmatrix} \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix} = 2x^4 - 4x^3 + 7x^2 - 4x + 2,$$

is non-negative. In fact,

$$f(x) \geq f(0.3768669139161389 \dots) \approx 1.312973699214175 \dots > 0.$$

Quiz

Is it possible to find $n \geq 1$ and $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \in \mathbb{R}^n$ such that

$$\|\mathbf{x}_1 - \mathbf{x}_2\| = \|\mathbf{x}_2 - \mathbf{x}_3\| = 1, \quad \|\mathbf{x}_1 - \mathbf{x}_3\| = 3?$$

Quiz

Is it possible to find $n \geq 1$ and $\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \in \mathbb{R}^n$ such that

$$\|\mathbf{x}_1 - \mathbf{x}_2\| = \|\mathbf{x}_2 - \mathbf{x}_3\| = 1, \quad \|\mathbf{x}_1 - \mathbf{x}_3\| = 3?$$

No, it is not possible as

$$\begin{aligned} \|\mathbf{x}_1 - \mathbf{x}_2\| &\leq \|\mathbf{x}_1 - \mathbf{x}_2 + \mathbf{x}_2 - \mathbf{x}_3\| \leq \\ &\leq \|\mathbf{x}_1 - \mathbf{x}_2\| + \|\mathbf{x}_2 - \mathbf{x}_3\|, \end{aligned}$$

(triangle inequality) but it is not true that $3 \leq 1 + 1 = 2$.

Properties of Pseudoinverses

Proposition

Let $A \in M(m \times n; \mathbb{R})$ be any matrix. Then $P = AA^+$ is a matrix of the orthogonal projection onto $\text{im}A$ and $Q = A^+A$ is a matrix of the orthogonal projection onto $\text{im}A^T$.

Proof.

Let $A = U\Sigma V^T$ be an SVD decomposition of A . Then

$$P = U\Sigma V^T V \Sigma^+ U^T = U_{:,1:r} U_{:,1:r}^T,$$

is symmetric where $r = r(A)$ and $U_{:,1:r}$ denotes first r columns of matrix U (orthonormal basis of $\text{im}A$). Moreover

$$P^2 = AA^+AA^+ = AA^+ = P.$$

Similarly for Q .



Properties of Pseudoinverses (continued)

Proposition

Let $A \in M(m \times n; \mathbb{R})$ be any matrix.

$$A^+ = (A^T A)^+ A^T, \quad A^+ = A^T (A A^T)^+.$$

Proof.

Let $A = U \Sigma V^T$ be an SVD decomposition of A . Then

$$A^T A = V \Sigma^2 V^T,$$

$$(A^T A)^+ = V (\Sigma^2)^+ V^T,$$

$$(A^T A)^+ A = V (\Sigma^2)^+ V^T V \Sigma U^T = A^+.$$

The second part is similar.



Properties of Pseudoinverses (continued)

Proposition

Let $A \in M(m \times n; \mathbb{R})$ be a matrix. If $r(A) = m$ (full row rank) then

$$A^+ = A^T(AA^T)^{-1}.$$

If $r(A) = n$ (full column rank) then

$$A^+ = (A^T A)^{-1} A^T.$$

Proof.

Follows from the above proposition (matrices AA^T and $A^T A$ are invertible).



Properties of Pseudoinverses (continued)

The following lemma will be subsequently used in the proof of Greville's conditions.

Proposition

Let $A, B \in M(m \times n; \mathbb{R})$ be any matrices. Then

$$A^T = A^+ A A^T,$$

$$B^T = B^T B B^+.$$

Proof.

Since A^+A is a matrix of (orthogonal) projection onto $\text{im}(A^T)$ and BB^+ is a matrix of (orthogonal) projection onto $\text{im}(B)$

$$A^T = A^+ A A^T,$$

$$B = B B^+ B.$$

Conjugating the last equation finishes the proof.



Inverse Law

Theorem (Greville)

Let $A \in M(m \times n; \mathbb{R})$, $B \in M(n \times k; \mathbb{R})$. If $(AB)^+ = B^+A^+$ then $\text{im}(A^T AB) \subset \text{im}(B)$ and $\text{im}(BB^T A^T) \subset \text{im}(A^T)$.

Proof.

By the above lemma applied to AB (the second case) using the main assumption

$$B^T A^T = B^T A^T A B B^+ A^+,$$

Multiplying on the right by $AA^T AB$ gives

$$B^T A^T A A^T A B = B^T A^T A B B^+ A^+ A A^T A B.$$

By the above lemma

$$B^T A^T A A^T A B = B^T A^T A B B^+ (A^+ A A^T) A B = B^T A^T A B B^+ A^T A B,$$

i.e.,

$$B^T A^T A (I - B B^+) A^T A B = 0.$$



Inverse Law(continued)

Proof.

$$B^T A^T A (I - BB^+) A^T AB = 0.$$

The middle matrix is idempotent and symmetric hence

$$\|(I - BB^+) A^T AB\|_2^2 = 0,$$

which is equivalent to

$$\text{im}(A^T AB) \subset \text{im}(B).$$

The rest is similar to the previous argument.



Inverse Law(continued)

In fact, the converse holds.

Theorem (Greville)

Let $A \in M(m \times n; \mathbb{R})$, $B \in M(n \times k; \mathbb{R})$. If $\text{im}(BB^T A^T) \subset \text{im}(A^T)$ and $\text{im}(A^T AB) \subset \text{im}(B)$ then $(AB)^+ = B^+ A^+$.

Proof.

The assumptions imply that

$$A^+ A B B^T A^T = B B^T A^T,$$

$$B B^+ A^T A B = A^T A B,$$

Multiplying the first equation on the right by $((AB)^T)^+$ and on the left by B^+ gives

$$B^+ A^+ A B B^T A^T ((AB)^T)^+ = B^+ B B^T A^T ((AB)^T)^+.$$

Inverse Law(continued)

Proof.

$$\begin{aligned}B^+A^+ABB^TA^T((AB)^T)^+ &= B^+BB^TA^T((AB)^T)^+. \\B^+A^+AB(AB)^T((AB)^T)^+ &= (B^+BB^T)A^T((AB)^T)^+.\end{aligned}$$

By the previous lemma this is equivalent to

$$B^+A^+AB = (AB)^T((AB)^T)^+,$$

therefore the matrix B^+A^+AB is symmetric.

Inverse Law(continued)

Proof.

Similarly, by multiplying

$$BB^+A^T AB = A^T AB,$$

on the left by $((A)^+)^T$

$$((A)^+)^T BB^+A^T AB = (((A)^+)^T A^T A)B,$$

$$((A)^+)^T BB^+A^T AB = AB.$$

Multiplying the above on the right by $(AB)^+$ and using on the left hand side $B^+ = (B^T B)^+ B^T$ gives

$$((A)^+)^T B(B^T B)^+ B^T A^T (AB)(AB)^+ = (AB)(AB)^+,$$

$$((A)^+)^T ((B)^+)^T (AB)^T = (AB)(AB)^+,$$

which, after conjugating side-wise implies that ABB^+A^+ is symmetric.

Inverse Law(continued)

Proof.

The first Penrose condition is easily verified.

$$\begin{aligned}ABB^+A^+AB &= AB(B^+A^+AB) = \\ &= AB(AB)^T((AB)^T)^+ = AB.\end{aligned}$$

Note that

$$\text{im}(BB^*A^*) \subset \text{im}(A^*) \implies \text{im}(BB^+A^+) \subset \text{im}(A^+).$$

($\text{im}(A^+) = \text{im}(A^*)$ and any eigenvector of BB^* is an eigenvector of BB^+ , moreover any linear combination of eigenvectors of BB^* corresponding to non-zero eigenvalues is an eigenvector of BB^+ .)

Inverse Law(continued)

Proof.

The second Penrose condition follows from $\text{im}(BB^+A^+) \subset \text{im}(A^+)$. Fix any vector u and let

$$v = B^+A^+ABB^+A^+u = B^+A^+A(BB^+A^+)u.$$

There exists vector w such that $(BB^+A^+)u = A^+w$, i.e.,

$$v = B^+A^+AA^+w = B^+A^+w = B^+BB^+A^+u = B^+A^+u.$$

Since vector u was arbitrary

$$B^+A^+ABB^+A^+ = B^+A^+.$$



Inverse Law(continued)

Remark

This also shows that condition $\text{im}(A^T AB) \subset \text{im}(B)$ implies conditions i), ii) and iii) for B^+A^+ .

Positive Semidefinite Block Matrix

Proposition

For any matrices

$A \in M(m \times m; \mathbb{R})$, $B \in M(n \times m; \mathbb{R})$, $C \in M(n \times n; \mathbb{R})$ where A and C are symmetric, let

$$M = \begin{bmatrix} A & B^T \\ B & C \end{bmatrix},$$

be a symmetric positive semidefinite matrix. Then

$$B^T = AA^+ B^T, \quad B = (CC^+)^T B.$$

Positive Semidefinite Block Matrix (continued)

Proof.

By spectral decomposition there exist $N \in M((m+n) \times (m+n); \mathbb{R})$ such that $M = N^T N$. Assume that $N = \begin{bmatrix} N_1 & N_2 \end{bmatrix}$, where $N_1 \in M((m+n) \times m; \mathbb{R})$, $N_2 \in M((m+n) \times n; \mathbb{R})$. Then

$$A = N_1^T N_1, \quad B^T = N_1^T N_2, \quad C = N_2^T N_2.$$

Moreover,

$$AA^+ B^T = (N_1^T N_1)(N_1^T N_1)^+ N_1^T N_2 = N_1^T N_2 = B^T,$$

as $(N_1^T N_1)(N_1^T N_1)^+$ is an orthogonal projection onto $\text{im}(N_1^T N_1) = \text{im}(N_1^T)$. Similarly,

$$(CC^+)^T B = (N_2^T N_2)^+ (N_2^T N_2) N_2^T N_1 = N_2^T N_1.$$



Schur Complement

Definition

For any matrices $A \in M(m \times m; \mathbb{R})$, $B \in M(m \times n; \mathbb{R})$, $C \in M(n \times m; \mathbb{R})$, $D \in M(n \times n; \mathbb{R})$ and the matrix

$$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix},$$

the **Schur complement** of matrix A with respect to M is

$$M|A = D - CA^+B.$$

Schur Complement (continued)

Proposition

A positive symmetric semidefinite matrix

$$M = \begin{bmatrix} A & B^T \\ B & C \end{bmatrix},$$

is conjugate to the matrix $\text{diag}(A, M|A)$, where $M|A = C - BA^+B^T$.

Proof.

$$\begin{aligned} & \begin{bmatrix} I & 0 \\ BA^+ & I \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & M|A \end{bmatrix} \begin{bmatrix} I & A^+B^T \\ 0 & I \end{bmatrix} = \\ & = \begin{bmatrix} A & 0 \\ BA^+A & M|A \end{bmatrix} \begin{bmatrix} I & A^+B^T \\ 0 & I \end{bmatrix} = \\ & = \begin{bmatrix} A & AA^+B^T \\ BA^+A & BA^+AA^+B^T + M|A \end{bmatrix} = \begin{bmatrix} A & AA^+B^T \\ BA^+A & C \end{bmatrix} = M. \end{aligned}$$

Schur Complement (continued)

Corollary

If a symmetric matrix

$$M = \begin{bmatrix} A & B^T \\ B & C \end{bmatrix},$$

is positive semidefinite then matrix A is positive semidefinite and the Schur complement $M|A$ is positive semidefinite. If matrix A is positive semidefinite and the Schur complement $M|A$ is positive semidefinite for symmetric matrix M and $BA^+A = B$ (for example when A is invertible) then M is positive semidefinite. Similar theorem is true for positive definite matrices.

Quiz (continued)

Is it possible to find $n \geq 1$ and $\mathbf{x}_0, \mathbf{x}_2, \dots, \mathbf{x}_5 \in \mathbb{R}^n$ such that (addition modulo 6)

$$\|\mathbf{x}_i - \mathbf{x}_{i \pm 1}\| = 1,$$

$$\|\mathbf{x}_i - \mathbf{x}_{i \pm 2}\| = \sqrt{3},$$

$$\|\mathbf{x}_i - \mathbf{x}_{i \pm 3}\| = 2?$$

Quiz (continued)

Is it possible to find $n \geq 1$ and $\mathbf{x}_0, \mathbf{x}_2, \dots, \mathbf{x}_5 \in \mathbb{R}^n$ such that (addition modulo 6)

$$\|\mathbf{x}_i - \mathbf{x}_{i \pm 1}\| = 1,$$

$$\|\mathbf{x}_i - \mathbf{x}_{i \pm 2}\| = \sqrt{3},$$

$$\|\mathbf{x}_i - \mathbf{x}_{i \pm 3}\| = 2?$$

Yes, it is. Those are vertices of a regular hexagon with sides of length 1 and $n = 2$.

Multidimensional Scaling

Definition

A symmetric non-negative matrix $D = [d_{ij}] \in M(n \times n; \mathbb{R}_{\geq 0})$ is called **Euclidean distance matrix** if there exist $m \geq 1$ and

$$\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^m,$$

such that

$$d_{ij} = \|\mathbf{x}_i - \mathbf{x}_j\|.$$

Definition

Let

$$H = I - n\mathbf{1}\mathbf{1}^T \in M(n \times n; \mathbb{R}),$$

be the **centering matrix**.

Multidimensional Scaling

Proposition

Let $D = [d_{ij}] \in M(n \times n; \mathbb{R}_{\geq 0})$ be a non-negative symmetric matrix. Let $A = [a_{ij}] \in M(n \times n; \mathbb{R})$ be a matrix given by the condition

$$a_{ij} = -\frac{1}{2}d_{ij}^2.$$

Let

$$B = HAH.$$

Multidimensional Scaling (continued)

Proposition

Then D is an Euclidean distance matrix if and only if matrix B is positive semidefinite. Moreover, in this case, let

$$\lambda_1 \geq \dots \geq \lambda_m > 0,$$

denote (all) positive eigenvalues of B (i.e., eigenvalue of multiplicity k appear exactly k times) with corresponding pairwise orthogonal eigenvectors w_1, \dots, w_m such that for $i = 1, \dots, m$

$$w_i \cdot w_i = \lambda_i.$$

Then $\mathbf{x}_i \in \mathbb{R}^m$ and \mathbf{x}_i lie in the rows of the matrix $\begin{bmatrix} v_1 & \dots & v_m \end{bmatrix}$. Moreover the barycenter of v_1, \dots, v_m is $\mathbf{0}$ and B is the Gram matrix of vectors v_1, \dots, v_m , i.e. $b_{ij} = v_i \cdot v_j$.

Example 1

Let

$$D = \begin{bmatrix} 0 & 1 & 3 \\ 1 & 0 & 1 \\ 3 & 1 & 0 \end{bmatrix}, \quad A = \begin{bmatrix} 0 & -\frac{1}{2} & -\frac{9}{2} \\ -\frac{1}{2} & 0 & -\frac{1}{2} \\ -\frac{9}{2} & -\frac{1}{2} & 0 \end{bmatrix}.$$

Then

$$B = HAH = \frac{1}{18} \begin{bmatrix} 38 & 5 & -43 \\ 5 & -10 & 5 \\ -43 & 5 & 38 \end{bmatrix},$$

which has eigenvalues $\lambda = -\frac{5}{6}$ or $\lambda = 0$ or $\lambda = \frac{9}{2}$, i.e. it is not positive semidefinite.

Example 2

Let

$$D = \begin{bmatrix} 0 & 1 & \sqrt{3} & 2 & \sqrt{3} & 1 \\ 1 & 0 & 1 & \sqrt{3} & 2 & \sqrt{3} \\ \sqrt{3} & 1 & 0 & 1 & \sqrt{3} & 2 \\ 2 & \sqrt{3} & 1 & 0 & 1 & \sqrt{3} \\ \sqrt{3} & 2 & \sqrt{3} & 1 & 0 & 1 \\ 1 & \sqrt{3} & 2 & \sqrt{3} & 1 & 0 \end{bmatrix},$$

$$A = \begin{bmatrix} 0 & -\frac{1}{2} & -\frac{3}{2} & -2 & -\frac{3}{2} & -\frac{1}{2} \\ -\frac{1}{2} & 0 & -\frac{1}{2} & -\frac{3}{2} & -2 & -\frac{3}{2} \\ -\frac{3}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & -\frac{3}{2} & -2 \\ -2 & -\frac{3}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} & -\frac{3}{2} \\ -\frac{3}{2} & -2 & -\frac{3}{2} & -\frac{1}{2} & 0 & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{3}{2} & -2 & -\frac{3}{2} & -\frac{1}{2} & 0 \end{bmatrix}.$$

Example 2 (continued)

Then

$$B = HAH = \frac{1}{2} \begin{bmatrix} 2 & 1 & -1 & -2 & -1 & 1 \\ 1 & 2 & 1 & -1 & -2 & -1 \\ -1 & 1 & 2 & 1 & -1 & -2 \\ -2 & -1 & 1 & 2 & 1 & -1 \\ -1 & -2 & -1 & 1 & 2 & 1 \\ 1 & -1 & -2 & -1 & 1 & 2 \end{bmatrix},$$

which has eigenvalues $\lambda = 0$ (of multiplicity 4) and $\lambda = 3$ (of multiplicity 2), i.e. it is positive semidefinite.

Example 2 (continued)

Moreover

$$V_{(3)} = \text{lin}((1, 0, -1, -1, 0, 1), (0, 1, 1, 0, -1, -1)),$$

which, after Gram-Schmidt process gives orthogonal basis

$$V_{(3)} = \text{lin}((1, 0, -1, -1, 0, 1), (1, 2, 1, -1, -2, -1)).$$

Let

$$w_1 = \frac{\sqrt{3}}{2}(1, 0, -1, -1, 0, 1),$$

$$w_2 = \frac{1}{2}(1, 2, 1, -1, -2, -1).$$

Then $w_1 \cdot w_2 = 0$ and $w_1 \cdot w_1 = w_2 \cdot w_2 = 3$.

Example 2 (continued)

Vectors $\mathbf{x}_0, \dots, \mathbf{x}_5 \in \mathbb{R}^2$ can be read from the rows of the matrix

$$\begin{bmatrix} w_1 & w_2 \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ 1 & 0 \\ \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -1 & 0 \\ -\frac{1}{2} & \frac{\sqrt{3}}{2} \end{bmatrix}.$$

Those are exactly the (complex) sixth roots of unity (clockwise).