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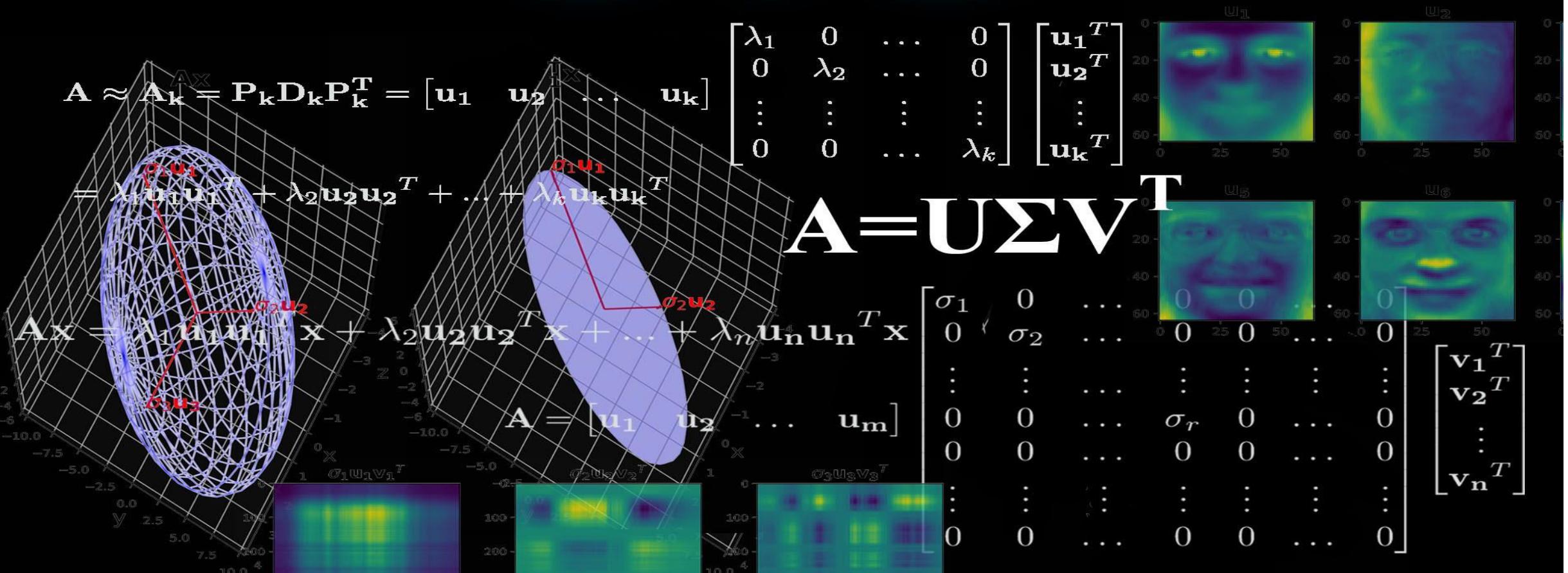


Unit 5 Singular Value Decomposition

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SVD



<https://towardsdatascience.com/understanding-singular-value-decomposition-and-its-application-in-data-science-388a54be95d>

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Importance of the method:



- Intimately related to the familiar theory of diagonalizing a symmetric matrix.
- Factorizes a matrix into 3 components.
- Has interesting algebraic properties.
- Gives further geometric and theoretical insights.
- Has many applications to data science.

Agenda for the chapter

- Tests for positive definiteness
- Positive Definite Matrices and Least Squares
- Semi definite Matrices
- Singular Value Decomposition
- Applications of the SVD.

Agenda for the class

- Quadratic form
- Examples on quadratic form
- Quadratic form – Going the other way.
- Quadratic forms for a non-symmetric matrix
- Graphs of quadratic forms
- Examples

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Recall

- If A is a real symmetric matrix of order n by n , then there exists an orthonormal matrix V whose columns are the eigenvectors of A and a diagonal matrix D , having its diagonal entries as the eigenvalues of A , such that : $A = VDV^T$
- The above process gives the eigenvalue decomposition of the matrix A .
- The singular value decomposition (SVD) is intimately related to the eigenvalue decomposition.

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Quadratic Form

Any $n \times n$ real symmetric matrix A determines a quadratic form q_A

in n variables by the formula

$$q_A(x_1, \dots, x_n) = \sum_{i=1}^n \sum_{j=1}^n a_{ij} x_i x_j = \mathbf{x}^T A \mathbf{x}.$$

Conversely, given a quadratic form in n variables, its coefficients can be arranged into an $n \times n$ symmetric matrix.

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Quadratic Form

✓ Note : $x^t A x$ is a scalar

$$\therefore x^T A x = (x_1 \ x_2 \ \dots \ x_m) \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1m} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2m} \\ \vdots & & & & \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mm} \end{bmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{pmatrix}$$

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Quadratic Form

$$\begin{aligned} & x_1(a_{11}x_1 + a_{12}x_2 + \dots + a_{1m}x_m) \\ & + x_2(a_{21}x_1 + a_{22}x_2 + \dots + a_{2m}x_m) \\ & + \vdots \\ & + x_m(a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mm}x_m) \\ & = \sum_{i \leq j}^m a_{ij} x_i x_j \end{aligned}$$

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Quadratic Form – Example 1

Let $\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. Compute $\mathbf{x}^T A \mathbf{x}$ for the following matrices.

a. $A = \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix}$

b. $A = \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix}$

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Quadratic Form - Example

Solution:

$$\text{a. } \mathbf{x}^T A \mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 4 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 4x_1 \\ 3x_2 \end{bmatrix} = 4x_1^2 + 3x_2^2.$$

$$\begin{aligned}\text{b. } \mathbf{x}^T A \mathbf{x} &= \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3x_1 - 2x_2 \\ -2x_1 + 7x_2 \end{bmatrix} \\ &= x_1(3x_1 - 2x_2) + x_2(-2x_1 + 7x_2) \\ &= 3x_1^2 - 2x_1x_2 - 2x_2x_1 + 7x_2^2 \\ &= 3x_1^2 - 4x_1x_2 + 7x_2^2\end{aligned}$$

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Quadratic Form – Example 2

$$A = \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix}$$

We could rewrite this in the form $Q(x) = 3x_1^2 - 4x_1x_2 + 7x_2^2$.

$$= x^T A x,$$

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Quadratic Form – Going the other way

Question: Is any function of the form $Q(x) = ax_1^2 + bx_1x_2 + cx_2^2$ a quadratic form?

Answer: Yes. Set $A = \begin{bmatrix} a & b/2 \\ b/2 & c \end{bmatrix}$.

Question: What about $Q(x) = 5x_1^2 + 3x_2^2 + 2x_3^2 - x_1x_2 + 8x_2x_3$?

Answer: Set $A = \begin{bmatrix} 5 & -1/2 & 0 \\ -1/2 & 3 & 4 \\ 0 & 4 & 2 \end{bmatrix}$.

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Quadratic Form – What if A isn't symmetric?

If A isn't symmetric, the function $Q(x) = x^T Ax$ is still a quadratic form:

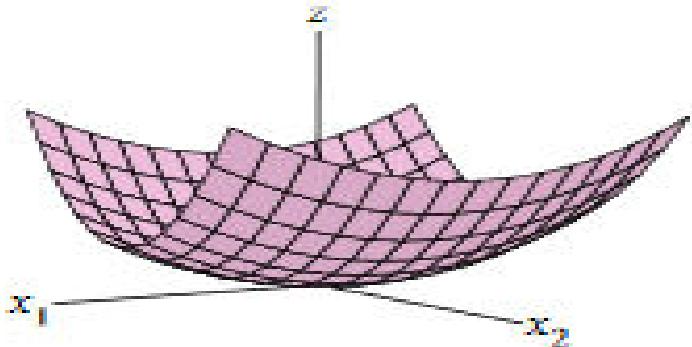
Define $\hat{A} = \frac{A+A^T}{2}$ then

$$\begin{aligned}x^T \hat{A} x &= x^T \left(\frac{A + A^T}{2} \right) x \\&= \frac{1}{2} (x^T A x + x^T A^T x) \\&= \frac{1}{2} (x^T A x + x^T A x) = x^T A x.\end{aligned}$$

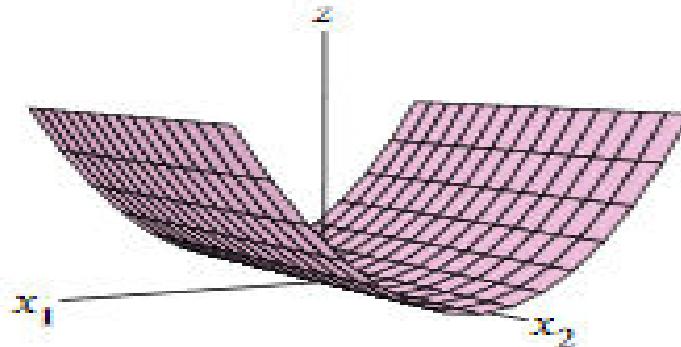
Because of this, it is safe to assume that A is symmetric when we examine quadratic forms.

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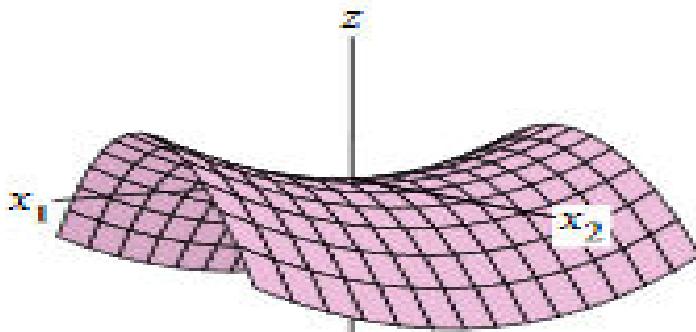
Graphs of Quadratic forms



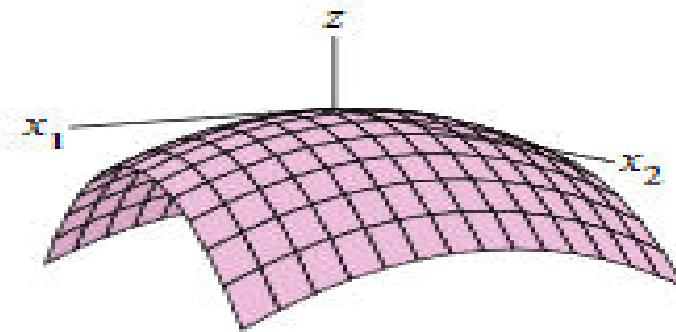
(a) $z = 3x_1^2 + 7x_2^2$



(b) $z = 3x_1^2$



(c) $z = 3x_1^2 - 7x_2^2$



(d) $z = -3x_1^2 - 7x_2^2$

Graphically, the graph $z = Q(x)$ is

- convex up if Q is positive definite,
- concave down if Q is negative definite,
- A “saddle” if Q is Indefinite.

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EXAMPLE

The quadratic form of $f(x,y) = ax^2 + 2abxy + by^2$
may be represented as $x^T A x$ where

$$x = \begin{bmatrix} x \\ y \end{bmatrix} ; \quad A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$



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Tests for Positive definiteness

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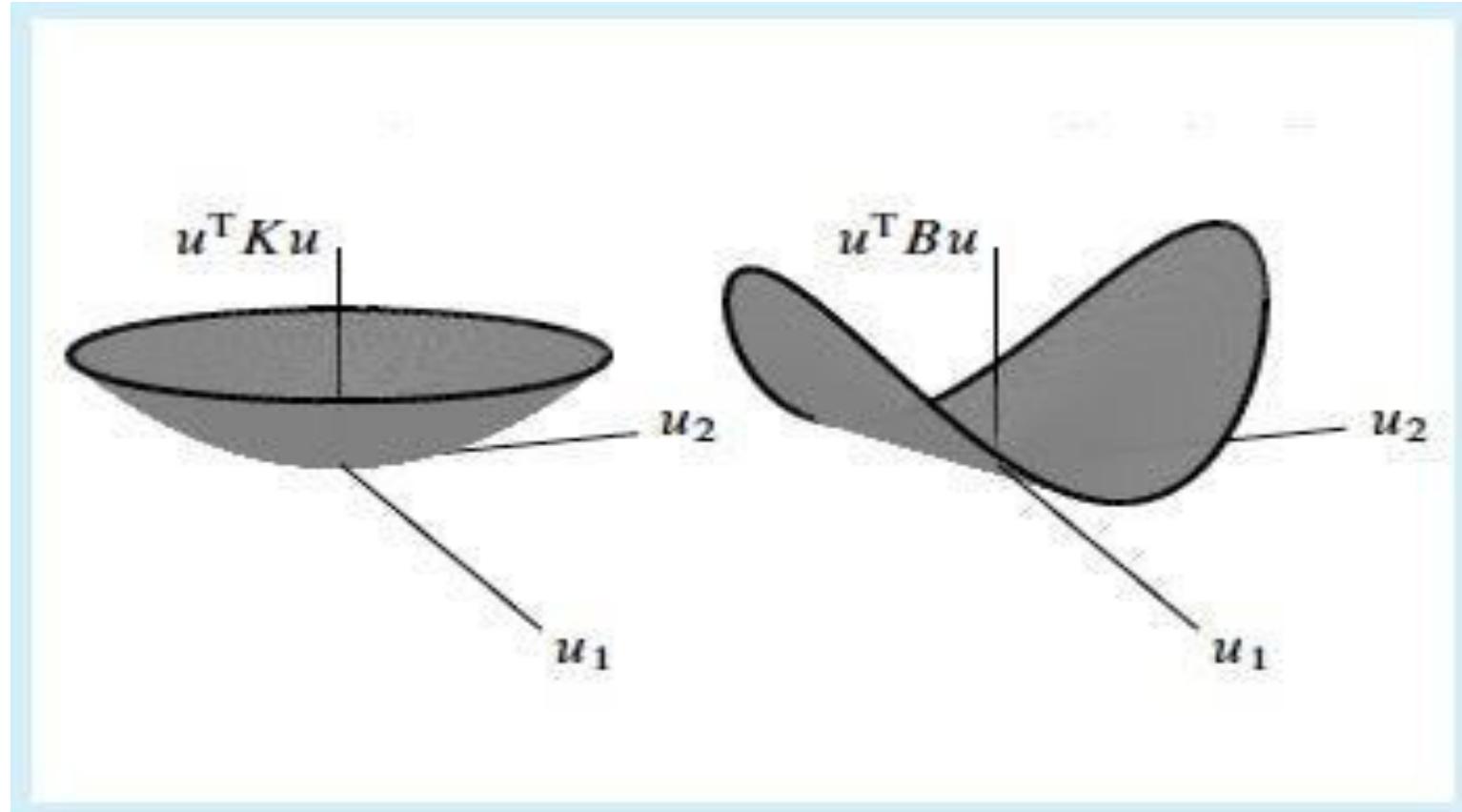
Agenda

- Quadratic form - Classification
- Positive Definite Matrix – $A+B$, $A^T A$
- Positivity of Eigenvalues
- Equivalent statements for positive definiteness
- Examples

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Quadratic Form: Classification

Positive definite and semidefinite: graphs of $x'Ax$.



<https://ocw.mit.edu/courses/mathematics/18-06sc-linear-algebra-fall-2011/positive-definite-matrices-and-applications/>

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Quadratic Form: Classification

Based on the sign of the quadratic form,
SVD can be classified into 3 categories:

Positive definite if $(\text{Quadratic form}) > 0$

Positive semi-definite if $(\text{Quadratic form}) \geq 0$

Negative definite if $(\text{Quadratic form}) < 0$

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$\tilde{A}^T A$ is Positive Definite

$\tilde{A}^T A$ is symmetric and square.

$$\text{Quadratic form: } \tilde{x}^T \tilde{A}^T A \tilde{x} = (\tilde{A}\tilde{x})^T (\tilde{A}\tilde{x}) = \|\tilde{A}\tilde{x}\|^2 > 0$$

$$A = \begin{bmatrix} 1 & 2 \\ 3 & -1 \end{bmatrix}; \quad \tilde{A}^T A = \begin{bmatrix} 1 & 3 \\ 2 & -1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 3 & -1 \end{bmatrix} = \begin{bmatrix} 10 & -1 \\ -1 & 5 \end{bmatrix}$$

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Positive Definiteness Of $A+B$

If A and B are positive definite, then so is $A+B$.

$$\boldsymbol{x}^T(A+B)\boldsymbol{x} = \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{x}^T B \boldsymbol{x} > 0$$

$$\therefore \boldsymbol{x}^T A \boldsymbol{x} > 0 \text{ and } \boldsymbol{x}^T B \boldsymbol{x} > 0 .$$

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POSITIVITY OF EIGENVALUES

Every eigenvalue of a positive definite matrix is positive.

Proof. Suppose A is a positive definite matrix. Let λ be an eigenvalue of A , and s be an eigenvector of A corresponding to λ . We have

$$As = \lambda s$$

It follows that

$$s^T As = \lambda(s^T s)$$

Hence

$$\lambda = \frac{s^T As}{s^T s} > 0$$

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POSITIVITY OF EIGENVALUES

A matrix is positive definite if every eigenvalue of the matrix is positive.

Proof. Suppose every eigenvalue of \mathbf{A} is positive. By spectral theorem, \mathbf{A} has an eigenvalue decomposition $\mathbf{A} = \mathbf{Q}\Lambda\mathbf{Q}^T$. It follows that

$$\mathbf{x}^T \mathbf{A} \mathbf{x} = \overbrace{\mathbf{x}^T \mathbf{Q}}^{y^T} \Lambda \overbrace{\mathbf{Q}^T \mathbf{x}}^{\mathbf{y}} = \mathbf{y}^T \Lambda \mathbf{y} = \sum_i \lambda_i y_i^2$$

Hence, the quadratic form $\mathbf{x}^T \mathbf{A} \mathbf{x}$ is positive for any $\mathbf{x} \neq 0$, and \mathbf{A} is positive definite.

Equivalent statements for Positive definiteness

There are many ways to say a matrix is positive definite.

- ① A is positive definite.
- ② Every eigenvalue of A is positive.
- ③ The determinant of every leading principal sub-matrices of A is positive.
- ④ A has full positive pivots.

What we have shown in the previous slides are

$$\textcircled{1} \Leftrightarrow \textcircled{2}$$

and

$$\textcircled{1} \Rightarrow \textcircled{3} \Rightarrow \textcircled{4} \Rightarrow \textcircled{1}$$

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Examples

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

The quadratic form of A is

The quadratic form of A is

$$\begin{aligned} \mathbf{x}^T A \mathbf{x} &= 2x_1^2 + 2x_2^2 + 2x_3^2 - 2x_1x_2 - 2x_2x_3 \\ &= 2\left(x_1 - \frac{1}{2}x_2\right)^2 + \frac{3}{2}\left(x_2 - \frac{2}{3}x_3\right)^2 + \frac{4}{3}x_3^2 \end{aligned}$$

The eigenvalues, the determinants, and the pivots are

$$\text{spectrum}(A) = \{2, 2 \pm \sqrt{2}\}, |A_1| = 2, |A_2| = 3, |A_3| = 4$$

$$A = \begin{bmatrix} 1 & 0 & 0 \\ -\frac{1}{2} & 1 & 0 \\ 0 & -\frac{2}{3} & 1 \end{bmatrix} \begin{bmatrix} 2 & & \\ & \frac{3}{2} & \\ & & \frac{4}{3} \end{bmatrix} \begin{bmatrix} 1 & -\frac{1}{2} & 0 \\ 0 & 1 & -\frac{2}{3} \\ 0 & 0 & 1 \end{bmatrix}$$

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EXAMPLE

For what numbers 'b' is the following matrix positive semi-definite?

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

Solution :

$$\begin{vmatrix} 2 & -1 & b \\ -1 & 2 & -1 \\ b & -1 & 2 \end{vmatrix} = -2b^2 + 2b + 4 \geq 0$$

$$\Rightarrow b^2 - b - 2 \leq 0$$

$$(b-1)(b+2) \leq 0 \quad -1 \leq b \leq 2$$



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- Semi Definite Matrices

Semi Definite Matrices

If A is a symmetric matrix then it is said to be positive semi-definite if

1) $x^T A x \geq 0 \quad \forall x$

2) All eigenvalues of A are greater than

or equal to zero i.e $\lambda_i \geq 0$.

- 3) None of the principal submatrices have negative determinants.
- 4) Pivots are non-negative (> 0)
- 5) There exists a matrix R , possibly with dependent columns such that $A = R^T R$

Example on semi-definite matrix

I. Test the matrix for positive semi-definiteness.

$$A = \begin{bmatrix} 5 & 2 & 1 \\ 2 & 2 & 2 \\ 1 & 2 & 5 \end{bmatrix}$$

Eigenvalues of A are $\lambda = 4, 4+2\sqrt{3}, 4-2\sqrt{3} > 0$

Example on semi-definite matrix

$$A \sim \begin{bmatrix} 5 & 2 & 1 \\ 0 & 6/5 & 8/5 \\ 0 & 8/5 & 24/5 \end{bmatrix} \sim \begin{bmatrix} 5 & 2 & 1 \\ 0 & 6/5 & 8/5 \\ 0 & 0 & 8/3 \end{bmatrix}$$

i) The pivots are: $0, \frac{6}{5}, \frac{8}{3} > 0$

ii) Determinants of submatrices: $|A_1| = 5 > 0$

Example on semi-definite matrix

$$3) |A_2| = \begin{vmatrix} 5 & 2 \\ 2 & 2 \end{vmatrix} = 6 > 0$$

$$4) |A_3| = 6 > 0$$

The above submatrices have positive determinants.

∴ The given matrix is positive definite.

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Example on semi-definite matrix

2) Test the positive semi-definiteness of the matrix

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

$$R_2 \rightarrow R_2 + \frac{1}{2} R_1$$

$$R_3 \rightarrow R_3 + \frac{1}{2} R_1$$

Example on semi-definite matrix

Solution : Characteristic Equation is $|A - \lambda I| = 0$

$$\Rightarrow \lambda^3 - 6\lambda^2 + 9\lambda - 18 = 0$$

$$\Rightarrow \lambda = 0, 3, 3 (\geq 0)$$

$$A \sim \left[\begin{array}{ccc} 2 & -1 & -1 \\ 0 & 3/2 & -3/2 \\ 0 & -3/2 & 3/2 \end{array} \right] \xrightarrow{R_3 \rightarrow R_3 + R_2} \left[\begin{array}{ccc} 2 & -1 & -1 \\ 0 & 3/2 & -3/2 \\ 0 & 0 & 0 \end{array} \right]$$

Example on semi-definite matrix

Pivots : $2, \frac{3}{2}, 0$ are non-negative

Determinants of the sub-matrices are:

$$|A_1| = 2 \geq 0 \quad ; \quad |A_3| = 0 \geq 0$$

$$|A_2| = 2 \geq 0$$

Hence the given matrix is positive semi-definite.



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- Least square problem – Normal equations.
- Positive Definiteness and the Least squares
- A simple example

The Normal Equations

Theorem: *Any solution x of the least squares problem is a solution of the linear system*

$$A^T A x = A^T b.$$

The system is nonsingular if and only if A has linearly independent columns.

Proof. • Since $b - Ax \in \ker(A^T)$, we have $A^T(b - Ax) = \mathbf{0}$ or

$$A^T A x = A^T b.$$

• $A^T A$ is nonsingular. Suppose $A^T A x = \mathbf{0}$ for some $x \in \mathbb{R}^n$. Then

$0 = x^T A^T A x = (Ax)^T A x = \|Ax\|_2^2$. Hence $Ax = \mathbf{0}$ which implies that $x = \mathbf{0}$ if and only if A has linearly independent columns.

The linear system $A^T A x = A^T b$ is called the **normal equations**.

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Positive Definite Matrices and Least Squares



We have learned that least square comes from projection :

$$b - p = e \Rightarrow A^T(b - A\hat{x}) = 0 \Rightarrow A^T A \hat{x} = A^T b$$

Consequently, only if $A^T A$ is invertible, then we can use linear regression to find approximate solutions $\hat{x} = (A^T A)^{-1} A^T b$ to unsolvable systems of linear equations.

According to the reasoning before, we know as long as all columns of $A_{m \times n}$ are mutual independent, then $A^T A$ is invertible. At the same time we ought to notice that the columns of A are guaranteed to be independent if they are orthogonal and even orthonormal.

In another prospective, if $A^T A$ is positive definite, then $A_{m \times n}$ has rank n (independent columns) and thus $A^T A$ is invertible.

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Positive Definite Matrices and Least Squares



Overall, if $A^T A$ is positive definite or invertible, then we can find approximate solutions of least square.

Find the function of the form

$$F(x) = c_1 + c_2 x \lg x + c_3 e^x$$

that is the best least-squares fit to the data points

$$(1, 1), (2, 1), (3, 3), (4, 8).$$

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Positive Definite Matrices and Least Squares



First we form the A matrix

$$A = \begin{pmatrix} 1 & 0 & e \\ 1 & 2 & e^2 \\ 1 & 3 \lg 3 & e^3 \\ 1 & 8 & e^4 \end{pmatrix}$$

We compute the pseudoinverse, then multiply it by y , to obtain the coefficient vector

$$c = \begin{pmatrix} 0.411741 \\ -0.20487 \\ 0.16546 \end{pmatrix}.$$

- Given $A^{m,n}$ and $b \in \mathbb{R}^m$.
- The system $Ax = b$ is **over-determined** if $m > n$.
- This system has a solution if $b \in \text{span}(A)$, the column space of A , but normally this is not the case and we can only find an approximate solution.
- A general approach is to choose a vector norm $\|\cdot\|$ and find x which minimizes $\|Ax - b\|$.
- We will only consider the Euclidian norm here.

- Given $A^{m,n}$ and $b \in \mathbb{R}^m$ with $m \geq n \geq 1$. The problem to find $x \in \mathbb{R}^n$ that minimizes $\|Ax - b\|_2$ is called the **least squares problem**.
- A minimizing vector x is called a **least squares solution** of $Ax = b$.
- Several ways to analyze:
- Quadratic minimization
- Orthogonal Projections
- SVD

- Define function $E : \mathbb{R}^n \rightarrow \mathbb{R}$ by $E(\mathbf{x}) = \|\mathbf{Ax} - \mathbf{b}\|_2^2$
- $E(\mathbf{x}) = (\mathbf{Ax} - \mathbf{b})^T(\mathbf{Ax} - \mathbf{b}) = \mathbf{x}^T \mathbf{Bx} - 2\mathbf{c}^T \mathbf{x} + \alpha$, where
- $\mathbf{B} := \mathbf{A}^T \mathbf{A}$, $\mathbf{c} := \mathbf{A}^T \mathbf{b}$ and $\alpha := \mathbf{b}^T \mathbf{b}$.
- \mathbf{B} is positive semidefinite and positive definite if \mathbf{A} has rank n .
- Since the Hessian $\mathbf{H}E(\mathbf{x}) := \left(\frac{\partial^2 E(\mathbf{x})}{\partial x_i \partial x_j} \right) = 2\mathbf{B}$ we can find minimum by setting partial derivatives equal zero.
- $\nabla E(\mathbf{x}) := \left(\frac{\partial E(\mathbf{x})}{\partial x_i} \right) = 2(\mathbf{Bx} - \mathbf{c}) = 0$
- **Normal equations** $\mathbf{A}^T \mathbf{Ax} = \mathbf{A}^T \mathbf{b}$.

A simple example



$$x_1 = 1 \quad x_1 = 1, \quad A = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \quad x = [x_1], \quad b = \begin{bmatrix} 1 \\ 1 \\ 2 \end{bmatrix},$$

- Quadratic minimization problem:

$$\|Ax - b\|_2^2 = (x_1 - 1)^2 + (x_1 - 1)^2 + (x_1 - 2)^2.$$

- Setting the first derivative with respect to x_1 equal to zero we obtain $2(x_1 - 1) + 2(x_1 - 1) + 2(x_1 - 2) = 0$ or $6x_1 - 8 = 0$ or $x_1 = 4/3$
- The second derivative is positive (it is equal to 6) and $x = 4/3$ is a global minimum.



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Agenda

- Singular value and singular vector
- Positivity of a Singular value
- Number of Singular values
- Singular value decomposition(SVD)
- Proofs of SVD
- Matrices and SVD
- Singular vectors and fundamental subspaces

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Singular Value and Singular Vector

A **singular value** of a real matrix A is the square root of a non-zero eigenvalue of $(A^T A)$.

It means to find the singular values of A , one needs to find the non-zero eigenvalues of $(A^T A)$.

Singular vector. If σ is a singular value of A , then there exists $v \neq 0$ such that

$$(A^T A) v = \sigma^2 v$$

Such a v is called a right singular vector of A with singular value σ . It is an eigenvector of $(A^T A)$ with eigenvalue σ^2 .

Positivity of a Singular Value

A singular value is always positive.

The matrix $(A^T A)$ is positive semi-definite:

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

so the eigenvalues of $(A^T A)$ must be non-negative, and the non-zero eigenvalues must be positive. Hence a singular value is positive.

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Number of Singular Values

A matrix of **rank** r has exactly r singular values.

Proof. Note $(\mathbf{A}^T \mathbf{A}) \mathbf{x} = 0 \Leftrightarrow \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} = 0 \Leftrightarrow \mathbf{A} \mathbf{x} = 0$, so

$\mathcal{N}(\mathbf{A}^T \mathbf{A}) = \mathcal{N}(\mathbf{A})$. Let \mathbf{A} be of order $m \times n$ with rank r .

Then $\dim \mathcal{N}(\mathbf{A}) = n - r = \dim \mathcal{N}(\mathbf{A}^T \mathbf{A})$. Matrix $(\mathbf{A}^T \mathbf{A})$ is non-defective, so the algebraic multiplicity of eigenvalue 0 is $(n - r)$. It follows that the total algebraic multiplicities of the non-zero eigenvalues of $(\mathbf{A}^T \mathbf{A})$ is

$$n - (n - r) = r$$

Notation. Singular values are denoted by $\sigma_1, \dots, \sigma_r$.

Singular Value Decomposition (SVD)

A real matrix can be decomposed by its singular values and singular vectors. This is called singular value decomposition.

A matrix of order $m \times n$ has SVD

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$$

where Σ is an $m \times n$ "diagonal" matrix with the singular values of \mathbf{A} as the leading diagonal elements, \mathbf{U} is an $m \times m$ orthogonal matrix with the eigenvectors of $(\mathbf{A}\mathbf{A}^T)$ as columns, and \mathbf{V} is an $n \times n$ orthogonal matrix with the eigenvectors of $(\mathbf{A}^T\mathbf{A})$ as columns.

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Proof of SVD

Let r be the rank of \mathbf{A} . Let $\sigma_1 \dots \sigma_r$ be the singular values of \mathbf{A} . Let $\mathbf{v}_1 \dots \mathbf{v}_r$ be orthonormal eigenvectors of $(\mathbf{A}^T \mathbf{A})$ with positive eigenvalues σ_i^2 and $\mathbf{u}_1 \dots \mathbf{u}_r$ be defined by $\mathbf{u}_i = \frac{\mathbf{A}\mathbf{v}_i}{\sigma_i}$. Note

$$(\mathbf{A}\mathbf{A}^T) \mathbf{u}_i = \frac{\mathbf{A}\mathbf{A}^T \mathbf{A}\mathbf{v}_i}{\sigma_i} = \frac{\mathbf{A}\sigma_i^2 \mathbf{v}_i}{\sigma_i} = \sigma_i^2 \mathbf{u}_i, \quad i = 1, \dots, r$$

So \mathbf{u}_i is an eigenvector of $(\mathbf{A}\mathbf{A}^T)$ with the same eigenvalue σ_i^2 . Let $\mathbf{v}_{r+1} \dots \mathbf{v}_n$ be orthonormal eigenvectors of $(\mathbf{A}^T \mathbf{A})$ with eigenvalue 0, and $\mathbf{u}_{r+1} \dots \mathbf{u}_m$ be eigenvectors of $(\mathbf{A}\mathbf{A}^T)$ with eigenvalue 0. Construct matrices \mathbf{U} and \mathbf{V} by

$$\mathbf{U} = \begin{bmatrix} \mathbf{u}_1 & \dots & \mathbf{u}_m \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \dots & \mathbf{v}_n \end{bmatrix}$$



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Agenda



- Proofs of SVD (Alternate proof)
- Matrices and SVD
- Singular vectors and fundamental subspaces

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Alternate proof of SVD

We show $\mathbf{U}^T \mathbf{A} \mathbf{V} = \Sigma$ which leads to SVD $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^T$. For $j = 1 \dots r$, we have $\mathbf{u}_j = \frac{\mathbf{A}\mathbf{v}_j}{\sigma_j}$, so $\mathbf{A}\mathbf{v}_j = \sigma_j \mathbf{u}_j$ and

$$(\mathbf{U}^T \mathbf{A} \mathbf{V})_{ij} = \mathbf{u}_i^T \mathbf{A} \mathbf{v}_j = \mathbf{u}_i^T (\sigma_j \mathbf{u}_j) = \sigma_j \delta_{ij}, \quad i = 1, \dots, m$$

For $j = r + 1 \dots n$, we have $(\mathbf{A}^T \mathbf{A}) \mathbf{v}_j = \mathbf{0}$, so $\mathbf{A}\mathbf{v}_j = \mathbf{0}$ and

$$(\mathbf{U}^T \mathbf{A} \mathbf{V})_{ij} = \mathbf{u}_i^T \mathbf{A} \mathbf{v}_j = 0, \quad i = 1, \dots, m$$

Combining the results, we get

$$\mathbf{U}^T \mathbf{A} \mathbf{V} = \Sigma$$

Hence

$$\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^T$$

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Matrices and SVD

For a matrix of order $m \times n$ with SVD $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$, the column vectors of \mathbf{U} (resp. \mathbf{V}) is an orthonormal basis of \mathbb{R}^m (resp. \mathbb{R}^n).

\mathbf{U} must be an eigenvector matrix of $\mathbf{A}\mathbf{A}^T$.

$$\mathbf{A}\mathbf{A}^T = (\mathbf{U}\Sigma\mathbf{V}^T)(\mathbf{V}\Sigma^T\mathbf{U}^T) = \mathbf{U} \overbrace{(\Sigma\Sigma^T)}^{\text{diagonal}} \mathbf{U}^T$$

Similarly, \mathbf{V} must be an eigenvector matrix of $\mathbf{A}^T\mathbf{A}$.

$$\mathbf{A}^T\mathbf{A} = (\mathbf{V}\Sigma^T\mathbf{U}^T)(\mathbf{U}\Sigma\mathbf{V}^T) = \mathbf{V} \overbrace{(\Sigma^T\Sigma)}^{\text{diagonal}} \mathbf{V}^T$$

The right (resp. left) singular vectors in an SVD of a matrix form an orthonormal basis of the row space (resp. column space) of the matrix.

Row space. $\{v_{r+1}, \dots, v_n\}$ contains eigenvectors of $(A^T A)$ with eigenvalue 0, so it is a basis of $\mathcal{N}(A^T A) = \mathcal{N}(A)$. This implies $\{v_1, \dots, v_r\}$ is a basis of the orthogonal complement of $\mathcal{N}(A)$, i.e. the row space of A .

Column space. We have $AV = U\Sigma$. The first r columns are

$$Av_i = \sigma_i u_i, \quad i = 1, \dots, r$$

So $\{u_1, \dots, u_r\}$ is a linearly independent set in the column space of A . Hence, it is a basis of $C(A)$.



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Agenda



- Problems on SVD
- SVD and Rank one matrices
- SVD and Pseudoinverse

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Problems on SVD

Find SVD of

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

The eigenvalues of

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

are $\lambda_1 = 3, \lambda_2 = 1, \lambda_3 = 0$. Hence the singular values of A are

$$\sigma_1 = \sqrt{3}, \sigma_2 = 1$$

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Problems on SVD

Orthonormal eigenvectors of $(A^T A)$ are

$$\mathbf{v}_1 = \frac{1}{\sqrt{6}} \begin{bmatrix} 1 \\ -2 \\ 1 \end{bmatrix}, \quad \mathbf{v}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \quad \mathbf{v}_3 = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

The corresponding left singular vectors of A are

$$\mathbf{u}_1 = \frac{\mathbf{Av}_1}{\sigma_1} = \frac{1}{\sqrt{2}} \begin{bmatrix} -1 \\ 1 \end{bmatrix}, \quad \mathbf{u}_2 = \frac{\mathbf{Av}_2}{\sigma_2} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

So

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T = \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \end{bmatrix}$$

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Rank One matrices and SVD

Every real matrix of rank r is the sum of r real matrices of rank 1 based on singular values and singular vectors.

By SVD

$$\begin{aligned} \mathbf{A} &= \mathbf{U}\Sigma\mathbf{V}^T = \sigma_1 \mathbf{u}_1 \mathbf{v}_1^T + \cdots + \sigma_r \mathbf{u}_r \mathbf{v}_r^T \\ &= \mathbf{A}_1 + \cdots + \mathbf{A}_r \end{aligned}$$

Image approximation. For an image of size 1000×1000 , a compression rate of 90% is achieved if 50 terms are used.

Let $A = U\Sigma V^T$ be an SVD of A . For a rectangular system of linear equations $Ax = b$, the least-squares solution with the minimum length is $x^+ = V\Sigma^+U^T b$.

Pseudo-inverse. The minimum-length least-squares solution can be written as $x^+ = A^+b$, where $A^+ = V\Sigma^+U^T$. A^+ is called the **pseudo-inverse** of A .

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SVD and Pseudoinverse



The Pseudoinverse of a matrix generalizes the notion of the inverse in a similar manner that SVD generalized the diagonalization of a matrix.

Not every matrix has an inverse, but every matrix has a pseudoinverse.

Computing the pseudoinverse from SVD is simple.

If $A = U\Sigma V^*$ then $A^+ = V\Sigma^+U^*$

where Σ^+ is formed from Σ by taking the reciprocal of all the non-zero elements, leaving all the zeros alone, and making the matrix the right shape: if Σ is an m by n matrix, then Σ^+ must be an n by m matrix.

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SVD and Pseudoinverse

Consider the matrix $A = \begin{bmatrix} 2 & -1 & 0 \\ 4 & 3 & -2 \end{bmatrix}$

The Singular value decomposition of A is

$$\begin{bmatrix} \frac{1}{\sqrt{26}} & -\frac{5}{\sqrt{26}} \\ \frac{5}{\sqrt{26}} & \frac{1}{\sqrt{26}} \end{bmatrix} \begin{bmatrix} \sqrt{30} & 0 & 0 \\ 0 & 2 & 0 \end{bmatrix} \begin{bmatrix} \frac{11}{\sqrt{195}} & \frac{7}{\sqrt{195}} & -\sqrt{\frac{5}{39}} \\ -\frac{3}{\sqrt{26}} & 2\sqrt{\frac{2}{13}} & -\frac{1}{\sqrt{26}} \\ \frac{1}{\sqrt{30}} & \sqrt{\frac{2}{15}} & \sqrt{\frac{5}{6}} \end{bmatrix}$$

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SVD and Pseudoinverse

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The Pseudoinverse may be computed from SVD using the definition explained earlier.

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More on Pseudoinverse A^\dagger .

- If A is square and nonsingular then $A^\dagger = A^{-1}$.
- A^\dagger is always defined.
- Thus A^\dagger is a generalization of usual inverse.
- If $B \in \mathbb{R}^{n,m}$ satisfies
 1. $ABA = A$
 2. $BAB = B$
 3. $(BA)^T = BA$
 4. $(AB)^T = AB$then $B = A^\dagger$.
- Thus A^\dagger is uniquely defined by these axioms.

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Example on Pseudoinverse A^\dagger .

Show that the pseudoinverse of $A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \\ 0 & 0 \end{bmatrix}$ is $B = \frac{1}{4} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix}$.

We have $BA = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ and $AB = \frac{1}{2} \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$. Thus

1. $ABA = A$
2. $BAB = B$
3. $(BA)^T = BA$
4. $(AB)^T = AB$

and hence $A^\dagger = B$.



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Agenda – Problems on SVD



- Example 1

Example 1. Find The singular value decomposition for the matrix:

$$A = \begin{bmatrix} 3 & 2 & 2 \\ 3 & 2 & -2 \end{bmatrix}$$

Solution: The singular value decomposition

of A is given by $A_{2 \times 3} = U_{2 \times 3} \sum_{2 \times 3} U^T_{2 \times 3}$

Where $U = A\bar{A}^T = \begin{bmatrix} 17 & 8 \\ 8 & 17 \end{bmatrix}$, a square
symmetric matrix.

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Agenda – Problems on SVD

Let $B = A\bar{A}^T$. Eigenvalues of B

can be found from: $|B - \lambda I| = 0$

$$\therefore \lambda_1 = 25, \lambda_2 = 9$$

Corresponding Eigenvectors are:

$$x_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \text{ and } x_2 = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

Note that x_1 and x_2 are orthogonal.

The orthonormal vectors are

$$u_1 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \quad \text{and} \quad u_2 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

$$\therefore U = [u_1 \ u_2] = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

Singular values are the square roots
of the eigenvalues .

$$\therefore \sigma_1 = \sqrt{\lambda_1} = \sqrt{25} = 5$$

and $\sigma_2 = \sqrt{\lambda_2} = \sqrt{9} = 3$

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Agenda – Problems on SVD

Defene $v_i = \frac{u_i^T A}{\sigma_i}$; $i = 1, 2$

$$\therefore v_1 = \frac{u_1^T A}{\sigma_1} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \end{bmatrix}^T$$

$$v_2 = \frac{u_2^T A}{\sigma_2} = \begin{bmatrix} -1/\sqrt{3} & 1/\sqrt{3} & -4/\sqrt{3} \end{bmatrix}^T$$

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Agenda – Problems on SVD

$$V = [v_1 \ v_2 \ v_3] = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{32} & * \\ 1/\sqrt{2} & 1/\sqrt{32} & * \\ 0 & -4/\sqrt{32} & * \end{bmatrix}$$

The 3rd vector v_3 must be orthogonal to both v_1 and v_2 .

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Agenda – Problems on SVD

$$\therefore \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{3}/2 & 1/\sqrt{3}/2 & -4/\sqrt{3}/2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Solving, we get $\frac{v_3}{\|v_3\|} = \frac{1}{\|v_3\|} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -2/\sqrt{3} \\ 2/\sqrt{3} \\ 1/\sqrt{3} \end{bmatrix}$

Agenda – Problems on SVD

Thus $V^T = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ -1/\sqrt{3}, 2 & 1/\sqrt{3}, 2 & -4/\sqrt{3}, 2 \\ -2/\sqrt{3} & 2/\sqrt{3} & 1/\sqrt{3} \end{bmatrix}$

The SVD is

$$A = U \sum V^T$$

where $\sum = \begin{bmatrix} \sqrt{5} & 0 & 0 \\ 0 & \sqrt{9} & 0 \end{bmatrix}_{2 \times 3}$.



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Agenda – Problems on SVD



- Example 2

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Agenda – Problems on SVD

Example 2. Find the SVD for $A = \begin{bmatrix} 1 & -1 \\ -2 & 2 \\ 2 & 2 \end{bmatrix}$

Soln : SVD: $A = U \Sigma V^T$

$$AA^T = \begin{bmatrix} 9 & -1 \\ -1 & 9 \end{bmatrix}$$

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Agenda – Problems on SVD

Eigenvalues of AA^T are

$\lambda_1 = 10, 8$ (arranged in increasing order)

Corresponding Eigenvectors are

$$x_1 = \begin{bmatrix} -1 \\ 1 \end{bmatrix} \text{ and } x_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

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Agenda – Problems on SVD

Clearly x_1 and x_2 are orthogonal.

$$V = \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = V^T$$

$$\Sigma = \begin{bmatrix} \sqrt{10} & 0 \\ 0 & \sqrt{8} \\ 0 & 0 \end{bmatrix}$$

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Agenda – Problems on SVD

$$u_i = \frac{A v_i}{\sigma_i} ; \quad i = 1, 2, 3 ; \quad \sigma_1 = \sqrt{10}, \sigma_2 = \sqrt{8}$$

$$u_1 = \begin{bmatrix} -1/\sqrt{5} \\ 2/\sqrt{5} \\ 0 \end{bmatrix} \quad u_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$u_1^T u_2 = 0 ; \quad u_1 \perp u_2 .$$

Agenda – Problems on SVD

Using orthogonality condition, u_3 can be obtained. Let $u_3 = \begin{bmatrix} x \\ y \\ z \end{bmatrix}$

$$\begin{bmatrix} -1/\sqrt{5} & 2/\sqrt{5} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

Agenda – Problems on SVD

∴ $u' = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}$, normalizing, we get

$$u_3 = \begin{bmatrix} 2/\sqrt{5} \\ 1/\sqrt{5} \\ 0 \end{bmatrix}; \quad u = \begin{bmatrix} -1/\sqrt{5} & 0 & 2/\sqrt{5} \\ 2/\sqrt{5} & 0 & 1/\sqrt{5} \\ 0 & 1 & 0 \end{bmatrix}$$

$$\therefore A = u \Sigma v^T$$



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Agenda – Applications of SVD

- Covariance of a matrix (2×2)
- Example on constructing covariance matrix

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Applications : Covariance of a 2x2 matrix



we can represent the covariance matrix by its eigenvectors and eigenvalues:

$$\Sigma \vec{v} = \lambda \vec{v}$$

where \vec{v} is an eigenvector of Σ , and λ is the corresponding eigenvalue.

Equation above

holds for each eigenvector-eigenvalue pair of matrix Σ . In the 2D case, we obtain

two eigenvectors and two eigenvalues. The system of two equations defined by equation
be represented efficiently using matrix notation:

$$\Sigma V = V L$$

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Applications : Covariance of a 2x2 matrix



This means that we can represent the covariance matrix as a function of its eigenvectors and eigenvalues:

$$\Sigma = V L V^{-1}$$

is called the eigendecomposition of the covariance matrix and can be obtained

using a [Singular Value Decomposition](#) algorithm. Whereas the eigenvectors represent the directions of the largest variance of the data, the eigenvalues represent the magnitude of this variance in those directions. In other words, V represents a rotation matrix, while \sqrt{L} represents a scaling matrix. The covariance matrix can thus be decomposed further as:

$$\Sigma = R S S R^{-1}$$

where $R = V$ is a rotation matrix and $S = \sqrt{L}$ is a scaling matrix.

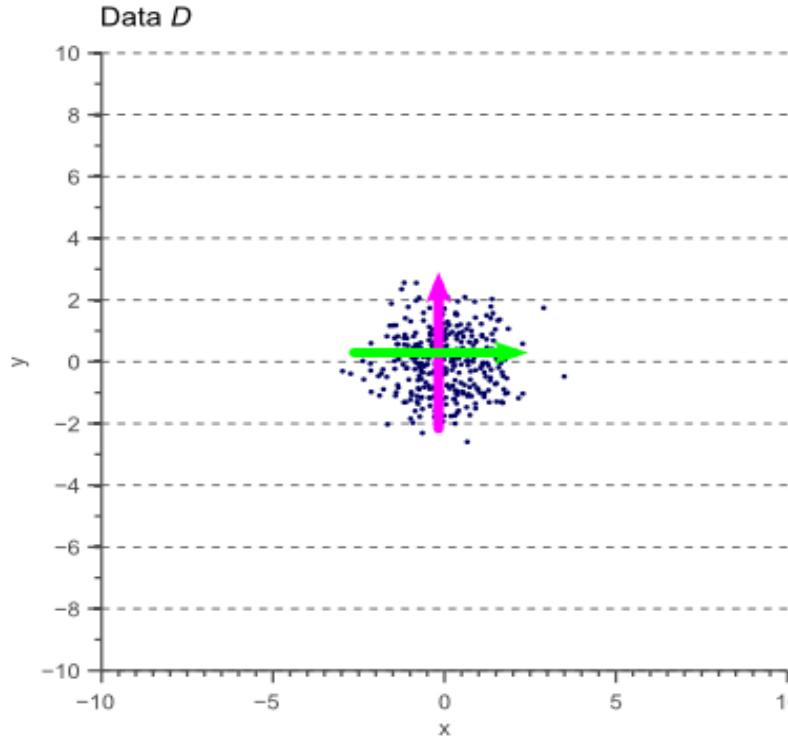
linear transformation $T = R S$. Since S is a diagonal scaling matrix, $S = S^\top$. Furthermore, since R is an orthogonal matrix, $R^{-1} = R^\top$. Therefore, $T^\top = (R S)^\top = S^\top R^\top = S R^{-1}$. The covariance matrix can thus be written as:

$$\Sigma = R S S R^{-1} = T T^\top,$$

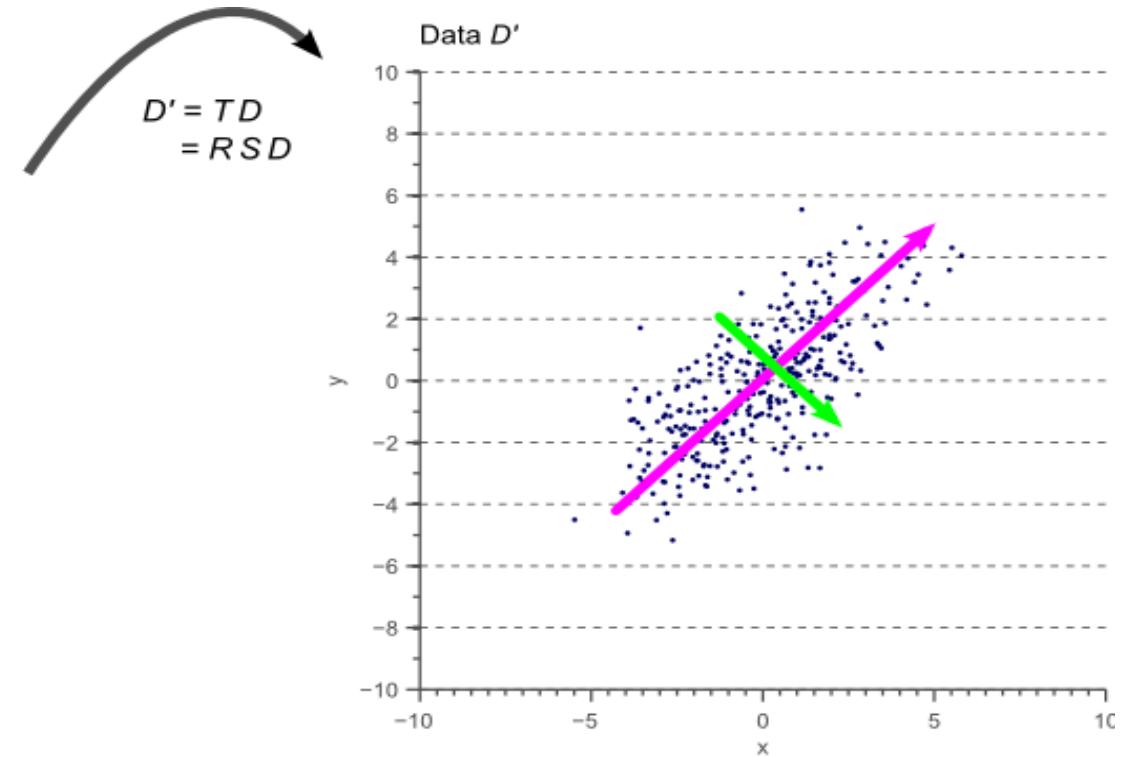
In other words, if we apply the linear transformation defined by $T = R S$ to the original data D shown by figure we obtain the rotated and scaled data D' with covariance matrix $T T^\top = \Sigma' = R S S R^{-1}$. This is illustrated by figure below

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Applications : Covariance of a 2x2 matrix



$$\Sigma = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



$$\Sigma' = \begin{bmatrix} 4.25 & 3.10 \\ 3.10 & 4.29 \end{bmatrix} = R S S R^{-1}$$

<https://www.visiondummy.com/wp-content/uploads/2014/04/lineartrans.png>

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Applications : Covariance of a 2x2 matrix



The covariance matrix represents a linear transformation of the original data.

The largest eigenvector, i.e. the

eigenvector with the largest corresponding eigenvalue, always points in the direction of the largest variance of the data and thereby defines its orientation. Subsequent eigenvectors are always orthogonal to the largest eigenvector due to the orthogonality of rotation matrices.

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Example: Covariance of a matrix

1) Find the covariance matrix given that :

$$X_1 = \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix} \quad X_2 = \begin{bmatrix} 4 \\ 2 \\ 13 \end{bmatrix} \quad X_3 = \begin{bmatrix} 7 \\ 8 \\ 1 \end{bmatrix}$$

and $X_4 = \begin{bmatrix} 8 \\ 4 \\ 5 \end{bmatrix}$

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Example: Covariance of a matrix

Step 1. Find the mean vector.

$$\text{Mean} = \frac{1}{n} [x_1 + x_2 + x_3 + x_4] = \begin{bmatrix} 5 \\ 4 \\ 5 \end{bmatrix} = M \text{ (say)}$$

Step 2: The mean deviation of the vectors x_i , $i=1,2,3,4$

$$\text{are } \hat{x}_i = x_i - M, \quad i=1,2,3,4.$$

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Example: Covariance of a matrix

Therefore $\hat{x}_1 = \begin{bmatrix} -4 \\ -2 \\ -4 \end{bmatrix}$, $\hat{x}_2 = \begin{bmatrix} -1 \\ -2 \\ 8 \end{bmatrix}$, $\hat{x}_3 = \begin{bmatrix} 2 \\ 4 \\ -4 \end{bmatrix}$ and

$$\hat{x}_4 = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix}.$$

Let the matrix $B = [\hat{x}_1 \ \hat{x}_2 \ \hat{x}_3 \ \hat{x}_4]$

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Example: Covariance of a matrix

Then,

$$B = \begin{bmatrix} -4 & -1 & 2 & 3 \\ -2 & -2 & 4 & 0 \\ -4 & 8 & -4 & 0 \end{bmatrix}$$

The covariance matrix is $S = \frac{1}{n-1} [BB^T]$

$$S = \frac{1}{3} \begin{bmatrix} 30 & 18 & 0 \\ 18 & 24 & -24 \\ 0 & -24 & 96 \end{bmatrix} = \begin{bmatrix} 10 & 6 & 0 \\ 6 & 8 & -8 \\ 0 & -8 & 32 \end{bmatrix}$$

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Example: Covariance of a matrix

2) The table below lists the weights and heights of 5 boys. Find the covariance matrix.

Boy : 1 2 3 4 5

Weight : 120 125 125 135 150

Height : 61 60 64 68 72

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Example: Covariance of a matrix

Solution: Let $X = \begin{pmatrix} \text{Weight} \\ \text{Height} \end{pmatrix}$

Mean of X is $M = \frac{1}{5} [x_1 + x_2 + x_3 + x_4 + x_5]$

$$\therefore M = \frac{1}{5} \begin{bmatrix} 650 \\ 325 \end{bmatrix} = \begin{bmatrix} 130 \\ 65 \end{bmatrix}$$

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Example: Covariance of a matrix

Let $\hat{x}_i = \bar{x}_i - M$, $i = 1, 2, 3, 4, 5$.

$$\therefore \hat{x}_1 = \begin{bmatrix} -10 \\ -4 \end{bmatrix}, \hat{x}_2 = \begin{bmatrix} -5 \\ -3 \end{bmatrix}, \hat{x}_3 = \begin{bmatrix} -5 \\ -1 \end{bmatrix}$$

$$\hat{x}_4 = \begin{bmatrix} 5 \\ 3 \end{bmatrix} \quad \text{and} \quad \hat{x}_5 = \begin{bmatrix} 15 \\ 7 \end{bmatrix}$$

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Example: Covariance of a matrix

Let $B = [\hat{x}_1 \hat{x}_2 \hat{x}_3 \hat{x}_4 \hat{x}_5]$

$$= \begin{bmatrix} -10 & -5 & -5 & 5 & 15 \\ -4 & -5 & -1 & 3 & 7 \end{bmatrix}_{2 \times 5}$$

$$S = \frac{1}{n-1} [BB^T] = \begin{bmatrix} 100 & \frac{190}{4} \\ \frac{190}{4} & 25 \end{bmatrix}$$



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