

Linear Algebra

Shan-Hung Wu
shwu@cs.nthu.edu.tw

Department of Computer Science,
National Tsing Hua University, Taiwan

Large-Scale ML, Fall 2016

Outline

- 1 Span & Linear Dependence
- 2 Norms
- 3 Eigendecomposition
- 4 Singular Value Decomposition
- 5 Traces and Determinant

Outline

- 1 **Span & Linear Dependence**
- 2 Norms
- 3 Eigendecomposition
- 4 Singular Value Decomposition
- 5 Traces and Determinant

Matrix Representation of Linear Functions

- A linear function (or map or transformation) $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ can be represented by a matrix \mathbf{A} , $\mathbf{A} \in \mathbb{R}^{m \times n}$, such that

$$f(\mathbf{x}) = \mathbf{A}\mathbf{x} = \mathbf{y}, \forall \mathbf{x} \in \mathbb{R}^n, \mathbf{y} \in \mathbb{R}^m$$

- $\text{span}(\mathbf{A}_{:,1}, \dots, \mathbf{A}_{:,n})$ is called the **column space** of \mathbf{A}
- $\text{rank}(\mathbf{A}) = \dim(\text{span}(\mathbf{A}_{:,1}, \dots, \mathbf{A}_{:,n}))$

System of Linear Equations

- Given A and y , solve x in $Ax = y$
- What kind of A that makes $Ax = y$ always have a solution?
 - Since $Ax = \sum_i x_i A_{:,i}$, the column space of A must contain \mathbb{R}^m , i.e.,
 $\mathbb{R}^m \subseteq \text{span}(A_{:,1}, \dots, A_{:,n})$
 - Implies $n \geq m$
- When does $Ax = y$ always have exactly one solution?
 - A has at most m columns; otherwise there is more than one x parametrizing each y
 - Implies $n = m$ and the columns of A are **linear independent** with each other
 - A^{-1} exists at this time, and $x = A^{-1}y$

Outline

- 1 Span & Linear Dependence
- 2 Norms**
- 3 Eigendecomposition
- 4 Singular Value Decomposition
- 5 Traces and Determinant

Vector Norms

- A **norm** of vectors is a function $\|\cdot\|$ that maps vectors to non-negative values satisfying
 - $\|\mathbf{x}\| = 0 \Rightarrow \mathbf{x} = \mathbf{0}$
 - $\|\mathbf{x} + \mathbf{y}\| \leq \|\mathbf{x}\| + \|\mathbf{y}\|$ (the triangle inequality)
 - $\|c\mathbf{x}\| = |c| \cdot \|\mathbf{x}\|, \forall c \in \mathbb{R}$
- E.g., the L^p norm

$$\|\mathbf{x}\|_p = \left(\sum_i |x_i|^p \right)^{1/p}$$

- L^2 (Euclidean) norm: $\|\mathbf{x}\| = (\mathbf{x}^\top \mathbf{x})^{1/2}$
 - L^1 norm: $\|\mathbf{x}\|_1 = \sum_i |x_i|$
 - Max norm: $\|\mathbf{x}\|_\infty = \max_i |x_i|$
- $\mathbf{x}^\top \mathbf{y} = \|\mathbf{x}\| \|\mathbf{y}\| \cos \theta$, where θ is the angle between \mathbf{x} and \mathbf{y}
 - \mathbf{x} and \mathbf{y} are **orthonormal** iff $\mathbf{x}^\top \mathbf{y} = 0$ (orthogonal) and $\|\mathbf{x}\| = \|\mathbf{y}\| = 1$ (unit vectors)

Matrix Norms

- Frobenius norm

$$\|A\|_F = \sqrt{\sum_{i,j} A_{i,j}^2}$$

- Analogous to the L^2 norm of a vector
- An **orthogonal matrix** is a square matrix whose column (resp. rows) are mutually orthonormal, i.e.,

$$A^\top A = I = AA^\top$$

- Implies $A^{-1} = A^\top$

Outline

- ① Span & Linear Dependence
- ② Norms
- ③ Eigendecomposition**
- ④ Singular Value Decomposition
- ⑤ Traces and Determinant

Decomposition

- Integers can be decomposed into prime factors
 - E.g., $12 = 2 \times 2 \times 3$
 - Helps identify useful properties, e.g., 12 is not divisible by 5
- Can we decompose matrices to identify information about their functional properties more easily?

Eigenvectors and Eigenvalues

- An *eigenvector* of a square matrix A is a non-zero vector \mathbf{v} such that multiplication by A alters only the scale of \mathbf{v} :

$$A\mathbf{v} = \lambda\mathbf{v},$$

where $\lambda \in \mathbb{R}$ is called the *eigenvalue* corresponding to this eigenvector

- If \mathbf{v} is an eigenvector, so is any its scaling $c\mathbf{v}, c \in \mathbb{R}, c \neq 0$
 - $c\mathbf{v}$ has the same eigenvalue
 - Thus, we usually look for unit eigenvectors

Eigendecomposition I

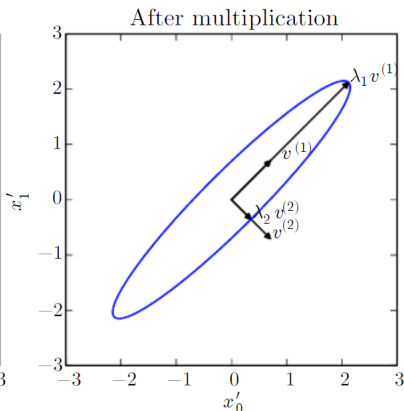
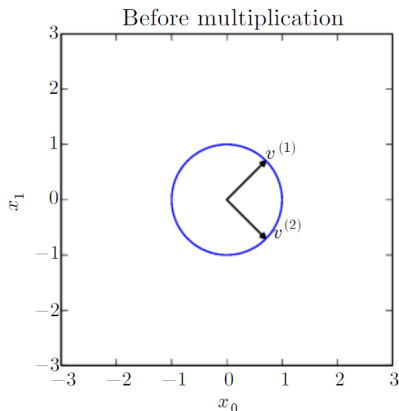
- Every *real symmetric* matrix $A \in \mathbb{R}^{n \times n}$ can be decomposed into

$$A = Q \text{diag}(\lambda) Q^\top$$

- $\lambda \in \mathbb{R}^n$ consists of real-valued eigenvalues (usually sorted in descending order)
- $Q = [\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}]$ is an orthogonal matrix whose columns are corresponding eigenvectors
- Eigendecomposition may not be unique
 - When any two or more eigenvectors share the same eigenvalue
 - Then any set of orthogonal vectors lying in their span are also eigenvectors with that eigenvalue
- What can we tell after decomposition?

Eigendecomposition II

- Because $\mathbf{Q} = [\mathbf{v}^{(1)}, \dots, \mathbf{v}^{(n)}]$ is an orthogonal matrix, we can think of \mathbf{A} as scaling space by λ_i in direction $\mathbf{v}^{(i)}$



Rayleigh's Quotient

Theorem (Rayleigh's Quotient)

Given a symmetric matrix $A \in \mathbb{R}^{n \times n}$, then $\forall \mathbf{x} \in \mathbb{R}^n$,

$$\lambda_{\min} \leq \frac{\mathbf{x}^\top A \mathbf{x}}{\mathbf{x}^\top \mathbf{x}} \leq \lambda_{\max},$$

where λ_{\min} and λ_{\max} are the smallest and largest eigenvalues of A .

- $\frac{\mathbf{x}^\top A \mathbf{x}}{\mathbf{x}^\top \mathbf{x}} = \lambda_i$ when \mathbf{x} is the corresponding eigenvector of λ_i

Singularity

- Suppose $A = Q \text{diag}(\lambda) Q^\top$, then $A^{-1} = Q \text{diag}(\lambda)^{-1} Q^\top$
- A is non-singular (invertible) iff none of the eigenvalues is zero

Positive Definite Matrices I

- A is **positive semidefinite** (denoted as $A \succeq \mathbf{O}$) iff its eigenvalues are all non-negative
 - $\mathbf{x}^\top A \mathbf{x} \geq 0$ for any \mathbf{x}
- A is **positive definite** (denoted as $A \succ \mathbf{O}$) iff its eigenvalues are all positive
 - Further ensures that $\mathbf{x}^\top A \mathbf{x} = 0 \Rightarrow \mathbf{x} = \mathbf{0}$
- Why these matter?

Positive Definite Matrices II

- A function f is **quadratic** iff it can be written as $f(x) = \frac{1}{2}x^\top Ax - b^\top x + c$, where A is symmetric
 - $x^\top Ax$ is called the **quadratic form**

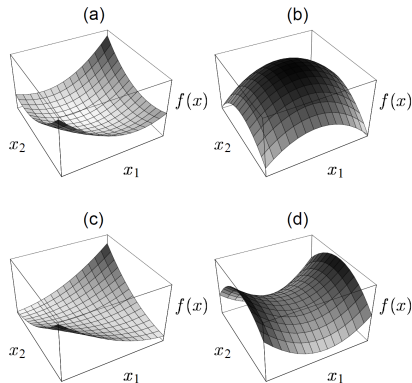


Figure: Graph of a quadratic form when A is a) positive definite; b) negative definite; c) positive semidefinite (singular); d) indefinite matrix.

Outline

- 1 Span & Linear Dependence
- 2 Norms
- 3 Eigendecomposition
- 4 Singular Value Decomposition**
- 5 Traces and Determinant

Singular Value Decomposition (SVD)

- Eigendecomposition requires square matrices. What if A is not square?
- Every real matrix $A \in \mathbb{R}^{m \times n}$ has a *singular value decomposition*:

$$A = UDV^\top,$$

where $U \in \mathbb{R}^{m \times m}$, $D \in \mathbb{R}^{m \times n}$, and $V \in \mathbb{R}^{n \times n}$

- U and V are orthogonal matrices, and their columns are called the *left-* and *right-singular vectors* respectively
- Elements along the diagonal of D are called the *singular values*
- Left-singular vectors of A are eigenvectors of AA^\top
- Right-singular vectors of A are eigenvectors of $A^\top A$
- Non-zero singular values of A are square roots of eigenvalues of AA^\top (or $A^\top A$)

Moore-Penrose Pseudoinverse I

- Matrix inversion is not defined for matrices that are not square
- Suppose we want to make a left-inverse $\mathbf{B} \in \mathbb{R}^{n \times m}$ of a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ so that we can solve a linear equation $\mathbf{A}\mathbf{x} = \mathbf{y}$ by left-multiplying each side to obtain $\mathbf{x} = \mathbf{B}\mathbf{y}$
 - If $m > n$, then it is possible to have no such \mathbf{B}
 - If $m < n$, then there could be multiple \mathbf{B} 's
- By letting $\mathbf{B} = \mathbf{A}^\dagger$ the *Moore-Penrose pseudoinverse*, we can make headway in these cases:
 - When $m = n$ and \mathbf{A}^{-1} exists, \mathbf{A}^\dagger degenerates to \mathbf{A}^{-1}
 - When $m > n$, \mathbf{A}^\dagger returns the \mathbf{x} for which $\mathbf{A}\mathbf{x}$ is closest to \mathbf{y} in terms of Euclidean norm $\|\mathbf{A}\mathbf{x} - \mathbf{y}\|$
 - When $m < n$, \mathbf{A}^\dagger returns the solution $\mathbf{x} = \mathbf{A}^\dagger \mathbf{y}$ with minimal Euclidean norm $\|\mathbf{x}\|$ among all possible solutions

Moore-Penrose Pseudoinverse II

- The Moore-Penrose pseudoinverse is defined as:

$$\mathbf{A}^\dagger = \lim_{\alpha \searrow 0} (\mathbf{A}^\top \mathbf{A} + \alpha \mathbf{I}_n)^{-1} \mathbf{A}^\top$$

- $\mathbf{A}^\dagger \mathbf{A} = \mathbf{I}$
- In practice, it is computed by $\mathbf{A}^\dagger = \mathbf{V} \mathbf{D}^\dagger \mathbf{U}^\top$, where $\mathbf{U} \mathbf{D} \mathbf{V}^\top = \mathbf{A}$
 - $\mathbf{D}^\dagger \in \mathbb{R}^{n \times m}$ is obtained by taking the inverses of its non-zero elements then taking the transpose

Outline

- 1 Span & Linear Dependence
- 2 Norms
- 3 Eigendecomposition
- 4 Singular Value Decomposition
- 5 Traces and Determinant**

Traces

- $\text{tr}(\mathbf{A}) = \sum_i \mathbf{A}_{i,i}$
- $\text{tr}(\mathbf{A}) = \text{tr}(\mathbf{A}^\top)$
- $\text{tr}(a\mathbf{A} + b\mathbf{B}) = a\text{tr}(\mathbf{A}) + b\text{tr}(\mathbf{B})$
- $\|\mathbf{A}\|_F^2 = \text{tr}(\mathbf{A}\mathbf{A}^\top) = \text{tr}(\mathbf{A}^\top\mathbf{A})$
- $\text{tr}(\mathbf{ABC}) = \text{tr}(\mathbf{BCA}) = \text{tr}(\mathbf{CAB})$
 - Holds even if the products have different shapes

Determinant I

- Determinant $\det(\cdot)$ is a function that maps a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ to a real value:

$$\det(\mathbf{A}) = \sum_i (-1)^{i+1} A_{1,i} \det(\mathbf{A}_{-1,-i}),$$

where $\mathbf{A}_{-1,-i}$ is the $(n-1) \times (n-1)$ matrix obtained by deleting the i -th row and j -th column

- $\det(\mathbf{A}^\top) = \det(\mathbf{A})$
- $\det(\mathbf{A}^{-1}) = 1/\det(\mathbf{A})$
- $\det(\mathbf{AB}) = \det(\mathbf{A}) \det(\mathbf{B})$
- $\det(\mathbf{A}) = \prod_i \lambda_i$
- What does it mean? $\det(\mathbf{A})$ can be also regarded as the *signed area of the image of the “unit square”*

Determinant II

- Let $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, we have $[1,0]A = [a,b]$, $[0,1]A = [c,d]$, and $\det(A) = ad - bc$

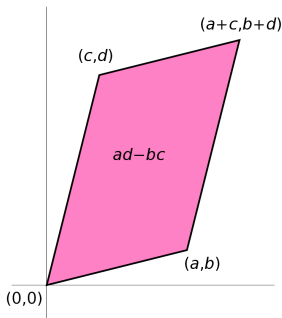


Figure: The area of the parallelogram is the absolute value of the determinant of the matrix formed by the images of the standard basis vectors representing the parallelogram's sides.

Determinant III

- The absolute value of the determinant can be thought of as a measure of how much multiplication by the matrix expands or contracts space
- If $\det(\mathbf{A}) = 0$, then space is contracted completely along at least one dimension
 - \mathbf{A} is invertible iff $\det(\mathbf{A}) \neq 0$
- If $\det(\mathbf{A}) = 1$, then the transformation is volume-preserving