Linear Algebra

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

Department of Computer Science, National Tsing Hua University, Taiwan

Large-Scale ML, Fall 2016

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Large-Scale ML, Fall 2016 1 / 26

Outline

1 Span & Linear Dependence

Norms

- 3 Eigendecomposition
- **4** Singular Value Decomposition
- **5** Traces and Determinant

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Outline

1 Span & Linear Dependence

2 Norms

3 Eigendecomposition

4 Singular Value Decomposition

5) Traces and Determinant

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Large-Scale ML, Fall 2016 3 / 26

Matrix Representation of Linear Functions

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

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

Matrix Representation of Linear Functions

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

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

Shan-Hung Wu (CS, NTHU)

• Given A and y, solve x in Ax = y

- Given A and y, solve x in Ax = y
- What kind of A that makes Ax = y always have a solution?

- Given A and y, solve x in Ax = y
- What kind of A that makes Ax = y always have a solution?
 - Since $A\mathbf{x} = \sum_i x_i A_{:,i}$, the column space of A must contain \mathbb{R}^m , i.e., $\mathbb{R}^m \subseteq span(A_{:,1}, \cdots, A_{:,n})$
 - Implies $n \ge m$

- Given A and y, solve x in Ax = y
- What kind of A that makes Ax = y always have a solution?
 - Since $A\mathbf{x} = \sum_i x_i A_{:,i}$, the column space of A must contain \mathbb{R}^m , i.e., $\mathbb{R}^m \subseteq span(A_{:,1}, \dots, A_{:,n})$
 - Implies $n \ge m$
- When does Ax = y always have exactly one solution?

- Given A and y, solve x in Ax = y
- What kind of A that makes Ax = y always have a solution?
 - Since $A\mathbf{x} = \Sigma_i x_i A_{:,i}$, the column space of A must contain \mathbb{R}^m , i.e., $\mathbb{R}^m \subseteq span(A_{:,1}, \cdots, A_{:,n})$
 - Implies $n \ge m$
- 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

- 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., $\mathbb{R}^m \subseteq span(A_{:,1}, \cdots, A_{:,n})$
 - Implies $n \ge m$
- 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 $x = A^{-1}y$

Shan-Hung Wu (CS, NTHU)

Outline

1 Span & Linear Dependence

2 Norms

3 Eigendecomposition

4 Singular Value Decomposition

5 Traces and Determinant

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Large-Scale ML, Fall 2016 6 / 26

Vector Norms

• A *norm* of vectors is a function $\|\cdot\|$ that maps vectors to non-negative values satisfying

•
$$\|\mathbf{x}\| = 0 \Rightarrow \mathbf{x} = \mathbf{0}$$

•
$$\|x+y\| \le \|x\| + \|y\|$$
 (the triangle inequality)

•
$$\|c\mathbf{x}\| = |c| \cdot \|\mathbf{x}\|, \forall c \in \mathbb{R}$$

Vector Norms

 A *norm* of vectors is a function || · || that maps vectors to non-negative values satisfying

•
$$\|\boldsymbol{x}\| = 0 \Rightarrow \boldsymbol{x} = \boldsymbol{0}$$

• $\|x+y\| \le \|x\| + \|y\|$ (the triangle inequality)

•
$$\|c\mathbf{x}\| = |c| \cdot \|\mathbf{x}\|, \forall c \in \mathbb{R}$$

• E.g., the L^p norm

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

- $L^2(\mathsf{Euclidean})$ norm: $||\mathbf{x}|| = (\mathbf{x}^\top \mathbf{x})^{1/2}$
- L^1 norm: $\|\boldsymbol{x}\|_1 = \sum_i |x_i|$
- Max norm: $\|\boldsymbol{x}\|_{\infty} = \max_i |x_i|$

Vector Norms

 A *norm* of vectors is a function || · || that maps vectors to non-negative values satisfying

•
$$\|\boldsymbol{x}\| = 0 \Rightarrow \boldsymbol{x} = \boldsymbol{0}$$

• $\|x+y\| \le \|x\| + \|y\|$ (the triangle inequality)

•
$$\|c\mathbf{x}\| = |c| \cdot \|\mathbf{x}\|, \forall c \in \mathbb{R}$$

• E.g., the L^p norm

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

- $L^2(\text{Euclidean})$ norm: $||\mathbf{x}|| = (\mathbf{x}^\top \mathbf{x})^{1/2}$
- L^1 norm: $\|\boldsymbol{x}\|_1 = \sum_i |x_i|$
- Max norm: $\|\boldsymbol{x}\|_{\infty} = \max_i |x_i|$

x[⊤]y = ||x|| ||y|| cos θ, where θ is the angle between x and y
x and y are orthonormal iff x[⊤]y = 0 (orthogonal) and ||x|| = ||y|| = 1 (unit vectors)

Shan-Hung Wu (CS, NTHU)

Matrix Norms

Frobenius norm

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

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

Shan-Hung Wu (CS, NTHU)

Outline

1 Span & Linear Dependence

2 Norms



4 Singular Value Decomposition

5 Traces and Determinant

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Large-Scale ML, Fall 2016 9 / 26

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

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 v such that multiplication by A alters only the scale of v :

$Av = \lambda v$,

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

Eigenvectors and Eigenvalues

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

$Av = \lambda v$,

where $\lambda \in \mathbb{R}$ is called the *eigenvalue* corresponding to this eigenvector • If ν is an eigenvector, so is any its scaling $c\nu, c \in \mathbb{R}, c \neq 0$

- cv has the same eigenvalue
- Thus, we usually look for unit eigenvectors

Eigendecomposition I

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

$$\boldsymbol{A} = \boldsymbol{Q} \operatorname{diag}(\lambda) \boldsymbol{Q}^{\mathsf{T}}$$

- $\lambda \in \mathbb{R}^n$ consists of real-valued eigenvalues (usually sorted in descending order)
- $Q = [\mathbf{v}^{(1)}, \cdots, \mathbf{v}^{(n)}]$ is an orthogonal matrix whose columns are corresponding eigenvectors

Eigendecomposition I

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

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

- $\lambda \in \mathbb{R}^n$ consists of real-valued eigenvalues (usually sorted in descending order)
- $Q = [v^{(1)}, \cdots, v^{(n)}]$ 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

Eigendecomposition I

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

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

- $\lambda \in \mathbb{R}^n$ consists of real-valued eigenvalues (usually sorted in descending order)
- $Q = [\mathbf{v}^{(1)}, \cdots, \mathbf{v}^{(n)}]$ 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 $Q = [v^{(1)}, \dots, v^{(n)}]$ is an orthogonal matrix, we can think of A as scaling space by λ_i in direction $v^{(i)}$



Rayleigh's Quotient

Theorem (Rayleigh's Quotient)

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

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

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

• $\frac{x^\top Px}{x^\top x} = \lambda_i$ when x is the corresponding eigenvector of λ_i

Shan-Hung Wu (CS, NTHU)

Singularity

• Suppose $A = Q \operatorname{diag}(\lambda) Q^{\top}$, then $A^{-1} = Q \operatorname{diag}(\lambda)^{-1} Q^{\top}$

Singularity

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

Positive Definite Matrices I

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

Positive Definite Matrices II

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

Positive Definite Matrices II

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

• $x^{\top}Ax$ is called the *quadratic form*

Positive Definite Matrices II

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

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Outline

1 Span & Linear Dependence

2 Norms

3 Eigendecomposition



5) Traces and Determinant

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Large-Scale ML, Fall 2016 18 / 26

Singular Value Decomposition (SVD)

• Eigendecomposition requires square matrices. What if A is not square?

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*

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*:

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^{\top},$$

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 $AA^{ op}$
- Right-singular vectors of A are eigenvectors of $A^{\top}A$
- Non-zero singular values of A are square roots of eigenvalues of $AA^{ op}$ (or $A^{ op}A$)

Shan-Hung Wu (CS, NTHU)

• Matrix inversion is not defined for matrices that are not square

- Matrix inversion is not defined for matrices that are not square
- Suppose we want to make a left-inverse $B \in \mathbb{R}^{n \times m}$ of a matrix $A \in \mathbb{R}^{m \times n}$ so that we can solve a linear equation Ax = y by left-multiplying each side to obtain x = By

- Matrix inversion is not defined for matrices that are not square
- Suppose we want to make a left-inverse $B \in \mathbb{R}^{n \times m}$ of a matrix $A \in \mathbb{R}^{m \times n}$ so that we can solve a linear equation Ax = y by left-multiplying each side to obtain x = By
 - If m > n, then it is possible to have no such **B**
 - If m < n, then there could be multiple **B**'s

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

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

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

Shan-Hung Wu (CS, NTHU)

• The Moore-Penrose pseudoinverse is defined as:

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

• $A^{\dagger}A = I$

• The Moore-Penrose pseudoinverse is defined as:

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

•
$$A^{\dagger}A = I$$

- ${} \bullet \;$ In practice, it is computed by $A^{\dagger} = V D^{\dagger} U^{\top}$, where $U D V^{\top} = A$
 - $D^{\dagger} \in \mathbb{R}^{n \times m}$ 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

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Large-Scale ML, Fall 2016 22 / 26

Traces

•
$$\operatorname{tr}(A) = \sum_{i} A_{i,i}$$

Shan-Hung Wu (CS, NTHU)

Linear Algebra

Large-Scale ML, Fall 2016 23 / 26

Traces

•
$$\operatorname{tr}(A) = \sum_{i} A_{i,i}$$

• $\operatorname{tr}(A) = \operatorname{tr}(A^{\top})$
• $\operatorname{tr}(aA + bB) = a\operatorname{tr}(A) + b\operatorname{tr}(B)$
• $||A||_{F}^{2} = \operatorname{tr}(AA^{\top}) = \operatorname{tr}(A^{\top}A)$
• $\operatorname{tr}(ABC) = \operatorname{tr}(BCA) = \operatorname{tr}(CAB)$

• Holds even if the products have different shapes

Shan-Hung Wu (CS, NTHU)

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

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

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

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

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

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

- $\det(A^{\top}) = \det(A)$
- $\det(\mathbf{A}^{-1}) = \frac{1}{\det(\mathbf{A})}$
- det(AB) = det(A) det(B)

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

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

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

- $\det(A^{\top}) = \det(A)$
- $\det(\mathbf{A}^{-1}) = \frac{1}{\det(\mathbf{A})}$
- det(AB) = det(A) det(B)
- det $(\mathbf{A}) = \prod_i \lambda_i$
- What does it mean?

Shan-Hung Wu (CS, NTHU)

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

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

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

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

Shan-Hung Wu (CS, NTHU)

• 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.

Shan-Hung Wu (CS, NTHU)

Linear Algebra

• The absolute value of the determinant can be thought of as a measure of how much multiplication by the matrix expands or contracts space

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

- 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 $\det(A)=0,$ then space is contracted completely along at least one dimension
 - A is invertible iff $\det(A) \neq 0$
- If det(A) = 1, then the transformation is volume-preserving