Mathematics for Machine Learning

Linear Algebra: Eigenvalues, Eigenvectors, Eigenspaces, Cholesky
 Decomposition & Diagonalization

Joseph Chuang-Chieh Lin

Department of Computer Science & Engineering, National Taiwan Ocean University

Fall 2025

Credits for the resource

- The slides are based on the textbooks:
 - Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.
 - Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra. Wiley. 2019.
- We could partially refer to the monograph: Francesco Orabona: A Modern Introduction to Online Learning. https://arxiv.org/abs/1912.13213

ML Math - Linear Algebra

• Matrix decomposition or matrix factorization.

- Matrix decomposition or matrix factorization.
- Three matrix decompositions will be introduced.

Outline

- Eigenvalues & Eigenvectors
- Cholesky Decomposition
- 3 Eigendecomposition & Diagonalization

Outline

Eigenvalues & Eigenvectors

- 2 Cholesky Decomposition
- 3 Eigendecomposition & Diagonalization

Characteristic Polynomial

Characteristic Polynomial

For $\lambda \in \mathbb{R}$ and a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$,

$$p_{\mathbf{A}}(\lambda) := \det(\mathbf{A} - \lambda \mathbf{I})$$

$$= (-1)^{n}(\lambda - \lambda_{1}) \cdots (\lambda - \lambda_{n})$$

$$= c_{0} + c_{1}\lambda + \cdots + c_{n-1}\lambda^{n-1} + (-1)^{n}\lambda^{n},$$

for $c_0, \ldots, c_{n-1} \in \mathbb{R}$, is called the characteristic polynomial of \boldsymbol{A} .

Note that

•
$$c_0 = \det(\mathbf{A})$$

Characteristic Polynomial

Characteristic Polynomial

For $\lambda \in \mathbb{R}$ and a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$,

$$p_{\mathbf{A}}(\lambda) := \det(\mathbf{A} - \lambda \mathbf{I})$$

$$= (-1)^{n}(\lambda - \lambda_{1}) \cdots (\lambda - \lambda_{n})$$

$$= c_{0} + c_{1}\lambda + \cdots + c_{n-1}\lambda^{n-1} + (-1)^{n}\lambda^{n},$$

for $c_0, \ldots, c_{n-1} \in \mathbb{R}$, is called the characteristic polynomial of \boldsymbol{A} .

Note that

- $c_0 = \det(\mathbf{A}) = \lambda_1 \cdot \lambda_2 \cdots \lambda_n$.
- $c_{n-1} = (-1)^{n-1} \operatorname{tr}(\mathbf{A})$

Characteristic Polynomial

Characteristic Polynomial

For $\lambda \in \mathbb{R}$ and a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$,

$$p_{\mathbf{A}}(\lambda) := \det(\mathbf{A} - \lambda \mathbf{I})$$

$$= (-1)^{n}(\lambda - \lambda_{1}) \cdots (\lambda - \lambda_{n})$$

$$= c_{0} + c_{1}\lambda + \cdots + c_{n-1}\lambda^{n-1} + (-1)^{n}\lambda^{n},$$

for $c_0, \ldots, c_{n-1} \in \mathbb{R}$, is called the characteristic polynomial of A.

Note that

- $c_0 = \det(\mathbf{A}) = \lambda_1 \cdot \lambda_2 \cdots \lambda_n$
- $c_{n-1} = (-1)^{n-1} \operatorname{tr}(\mathbf{A}) = (-1)^{n-1} (\lambda_1 + \lambda_2 + \dots + \lambda_n).$





ML Math - Linear Algebra Eigenvalues & Eigenvectors

Example

Given
$$\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 8 & -1 \end{bmatrix}$$
,

$$\det(\mathbf{A} - \lambda \mathbf{I}) = \begin{vmatrix} 3 - \lambda & 0 \\ 8 & -1 - \lambda \end{vmatrix} = (3 - \lambda)(-1 - \lambda).$$

Joseph C. C. Lin (CSE, NTOU, TW)

Example

Given
$$\mathbf{A} = \begin{bmatrix} 3 & 0 \\ 8 & -1 \end{bmatrix}$$
,

$$\det(\mathbf{A} - \lambda \mathbf{I}) = \begin{vmatrix} 3 - \lambda & 0 \\ 8 & -1 - \lambda \end{vmatrix} = (3 - \lambda)(-1 - \lambda).$$

Given
$$\mathbf{B} = \left| \begin{array}{ccc} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 4 & -17 & 8 \end{array} \right|,$$

$$\det(\boldsymbol{B} - \lambda \boldsymbol{I}) = \begin{vmatrix} -\lambda & 1 & 0 \\ 0 & -\lambda & 1 \\ 4 & -17 & 8 - \lambda \end{vmatrix} = -\lambda^3 + 8\lambda^2 - 17\lambda + 4.$$

◆ロト ◆個ト ◆ 恵ト ◆ 恵 ・ り へ ○

Eigenvalue Equation

Eigenvalues & Eigenvectors

Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ be a square matrix. Then

- $\lambda \in \mathbb{R}$ is an eigenvalue of **A** and
- $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ is the corresponding eigenvector of A

if $\mathbf{A}\mathbf{x} = \lambda \mathbf{x}$.

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \iff (\mathbf{A} - \lambda \mathbf{I})\mathbf{x} = \mathbf{0}$$

Equivalent statements:

- λ is an eigenvalue of $\mathbf{A} \in \mathbb{R}^{n \times n}$.
- There exists an $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ with $\mathbf{A}\mathbf{x} = \lambda \mathbf{x}$ (i.e., $(\mathbf{A} \lambda \mathbf{I}_n)\mathbf{x} = \mathbf{0}$) that can be solved non-trivially (i.e., $\mathbf{x} \neq \mathbf{0}$).
- $\operatorname{rank}(\boldsymbol{A} \lambda \boldsymbol{I}_n) < n$.
- $\bullet \det(\boldsymbol{A} \lambda \boldsymbol{I}_n) = 0.$

Remark

• Eigenvectors are NOT unique.

Remark

- Eigenvectors are NOT unique.
- Suppose **x** is an eigenvector of **A** w.r.t. eigenvalue λ , then for any $c \in \mathbb{R} \setminus \mathbf{0}$ }

$$\mathbf{A}(c\mathbf{x}) = c\mathbf{A}\mathbf{x} = c\lambda\mathbf{x} = \lambda(c\mathbf{x}).$$

Theorem

 $\lambda \in \mathbb{R}$ is an eigenvalue of $\mathbf{A} \in \mathbb{R}^{n \times n}$ if and only if λ is a root of the characteristic polynomial $p_{\mathbf{A}}(\lambda)$ of \mathbf{A} .

Theorem

 $\lambda \in \mathbb{R}$ is an eigenvalue of $\mathbf{A} \in \mathbb{R}^{n \times n}$ if and only if λ is a root of the characteristic polynomial $p_{\mathbf{A}}(\lambda)$ of \mathbf{A} .

Algebraic Multiplicity

Suppose that matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ has an eigenvalue λ_i . The algebraic multiplicity of λ_i is the number of times the root appears in the characteristic polynomial.

• Denoted by $am(\lambda_i)$

Theorem

 $\lambda \in \mathbb{R}$ is an eigenvalue of $\mathbf{A} \in \mathbb{R}^{n \times n}$ if and only if λ is a root of the characteristic polynomial $p_{\mathbf{A}}(\lambda)$ of \mathbf{A} .

Algebraic Multiplicity

Suppose that matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ has an eigenvalue λ_i . The algebraic multiplicity of λ_i is the number of times the root appears in the characteristic polynomial.

• Denoted by $am(\lambda_i)$

Eigenspace

For $\mathbf{A} \in \mathbb{R}^{n \times n}$, the set of all eigenvectors of \mathbf{A} associated with the eigenvalue λ spans the eigenspace of \mathbf{A} (denoted by E_{λ}).

Geometric Multiplicity

 $\dim(E_{\lambda})$ is called the geometric multiplicity of λ .

• Denoted by $gm(\lambda)$.

Eigenspectrum (Spectrum)

The set of all eigenvalues of \boldsymbol{A} is called the eigenspectrum (or spectrum) of \boldsymbol{A} .

Relation b/w am(λ) & gm(λ)

Geometric multiplicity Algebraic multiplicity

Given $\mathbf{A} \in \mathbb{R}^{n \times n}$ and assume that λ is an eigenvalue of \mathbf{A} , then

$$gm(\lambda) \leq am(\lambda)$$
.

• Assume that $\dim(E_{\lambda}) = k \le n$ and let $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is a basis of E_{λ} such that $\mathbf{v}_1, \dots, \mathbf{v}_k$ are eigenvectors w.r.t. λ .

Relation b/w am(λ) & gm(λ)

Geometric multiplicity ≤ Algebraic multiplicity

Given $\mathbf{A} \in \mathbb{R}^{n \times n}$ and assume that λ is an eigenvalue of \mathbf{A} , then

$$gm(\lambda) \leq am(\lambda)$$
.

- Assume that $\dim(E_{\lambda}) = k \le n$ and let $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is a basis of E_{λ} such that $\mathbf{v}_1, \dots, \mathbf{v}_k$ are eigenvectors w.r.t. λ .
- $\exists \mathbf{v}_{k+1}, \dots, \mathbf{v}_n$ such that $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ is a basis of \mathbb{R}^n .

Relation b/w am(λ) & gm(λ)

Geometric multiplicity Algebraic multiplicity

Given $\mathbf{A} \in \mathbb{R}^{n \times n}$ and assume that λ is an eigenvalue of \mathbf{A} , then

$$gm(\lambda) \leq am(\lambda)$$
.

- Assume that $\dim(E_{\lambda}) = k \leq n$ and let $\{\mathbf{v}_1, \dots, \mathbf{v}_k\}$ is a basis of E_{λ} such that $\mathbf{v}_1, \dots, \mathbf{v}_k$ are eigenvectors w.r.t. λ .
- $\exists \mathbf{v}_{k+1}, \dots, \mathbf{v}_n$ such that $\{\mathbf{v}_1, \dots, \mathbf{v}_n\}$ is a basis of \mathbb{R}^n .
- Denote by $P = [U \ V]$ for $U = [\mathbf{v}_1 \cdots \mathbf{v}_k]$ and $V = [\mathbf{v}_{k+1} \cdots \mathbf{v}_n]$ (note: P is invertible).

◆ロト ◆団ト ◆豆 ◆ ◆豆 ◆ 豆 ・ 夕 へ ○

• : P is invertible \Rightarrow Let $P^{-1} = \begin{bmatrix} X \\ Y \end{bmatrix}$, where $X \in \mathbb{R}^{k \times n}$ and $Y \in \mathbb{R}^{(n-k) \times n}$.

- : P is invertible \Rightarrow Let $P^{-1} = \begin{bmatrix} X \\ Y \end{bmatrix}$, where $X \in \mathbb{R}^{k \times n}$ and $Y \in \mathbb{R}^{(n-k) \times n}$.
- Then,

$$\left[\begin{array}{cc} \textbf{\textit{I}}_k & \textbf{\textit{O}} \\ \textbf{\textit{O}} & \textbf{\textit{I}}_{n-k} \end{array}\right] = \textbf{\textit{P}}^{-1}\textbf{\textit{P}} = \left[\begin{array}{cc} \textbf{\textit{X}} \\ \textbf{\textit{Y}} \end{array}\right] \left[\textbf{\textit{U}} \quad \textbf{\textit{V}}\right] = \left[\begin{array}{cc} \textbf{\textit{XU}} & \textbf{\textit{XV}} \\ \textbf{\textit{YU}} & \textbf{\textit{YV}} \end{array}\right]$$

- : P is invertible \Rightarrow Let $P^{-1} = \begin{bmatrix} X \\ Y \end{bmatrix}$, where $X \in \mathbb{R}^{k \times n}$ and $Y \in \mathbb{R}^{(n-k) \times n}$.
- Then,

$$\left[\begin{array}{cc} \boldsymbol{I}_k & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I}_{n-k} \end{array}\right] = \boldsymbol{P}^{-1}\boldsymbol{P} = \left[\begin{array}{cc} \boldsymbol{X} \\ \boldsymbol{Y} \end{array}\right] \left[\boldsymbol{U} \quad \boldsymbol{V}\right] = \left[\begin{array}{cc} \boldsymbol{X}\boldsymbol{U} & \boldsymbol{X}\boldsymbol{V} \\ \boldsymbol{Y}\boldsymbol{U} & \boldsymbol{Y}\boldsymbol{V} \end{array}\right]$$

• Note that $\mathbf{A}\mathbf{U} = \mathbf{A}[\mathbf{v}_1 \cdots \mathbf{v}_k] = [\mathbf{A}\mathbf{v}_1 \cdots \mathbf{A}\mathbf{v}_k] = [\lambda \mathbf{v}_1 \cdots \lambda \mathbf{v}_k] = \lambda \mathbf{U}$.

$$P^{-1}AP = \begin{bmatrix} X \\ Y \end{bmatrix}A[U \ V] = \begin{bmatrix} XAU \ YAU \ YAV \end{bmatrix}$$

$$P^{-1}AP = \begin{bmatrix} X \\ Y \end{bmatrix} A[U \ V] = \begin{bmatrix} XAU & XAV \\ YAU & YAV \end{bmatrix}$$
$$= \begin{bmatrix} \lambda XU & XAV \\ \lambda YU & YAV \end{bmatrix} = \begin{bmatrix} \lambda I_k & XAV \\ 0 & YAV \end{bmatrix}$$

$$P^{-1}AP = \begin{bmatrix} X \\ Y \end{bmatrix} A[U \ V] = \begin{bmatrix} XAU \ XAV \\ YAU \ YAV \end{bmatrix}$$
$$= \begin{bmatrix} \lambda XU \ XAV \\ \lambda YU \ YAV \end{bmatrix} = \begin{bmatrix} \lambda I_k \ XAV \\ 0 \ YAV \end{bmatrix}$$

$$\det(\mathbf{P}^{-1}\mathbf{A}\mathbf{P} - z\mathbf{I}) = \det\begin{bmatrix} \lambda \mathbf{I}_k - z\mathbf{I}_k & \mathbf{X}\mathbf{A}\mathbf{V} \\ \mathbf{O} & \mathbf{Y}\mathbf{A}\mathbf{V} - z\mathbf{I}_{n-k} \end{bmatrix}$$

$$P^{-1}AP = \begin{bmatrix} X \\ Y \end{bmatrix} A[U \ V] = \begin{bmatrix} XAU \ XAV \\ YAU \ YAV \end{bmatrix}$$
$$= \begin{bmatrix} \lambda XU \ XAV \\ \lambda YU \ YAV \end{bmatrix} = \begin{bmatrix} \lambda I_k \ XAV \\ 0 \ YAV \end{bmatrix}$$

$$\det(\mathbf{P}^{-1}\mathbf{A}\mathbf{P} - z\mathbf{I}) = \det\begin{bmatrix} \lambda \mathbf{I}_k - z\mathbf{I}_k & \mathbf{X}\mathbf{A}\mathbf{V} \\ \mathbf{0} & \mathbf{Y}\mathbf{A}\mathbf{V} - z\mathbf{I}_{n-k} \end{bmatrix}$$
$$= (\lambda - z)^k \det(\mathbf{Y}\mathbf{A}\mathbf{V} - z\mathbf{I}_{n-k}).$$

• Note: $\det(\mathbf{A} - z\mathbf{I}) = \det(\mathbf{P}^{-1}\mathbf{A}\mathbf{P} - z\mathbf{I})$.

◆□▶◆圖▶◆臺▶◆臺▶ 臺 釣魚◎

Remark

$$P^{-1}AP - zI = P^{-1}AP - zP^{-1}P$$

$$= P^{-1}AP - P^{-1}(zI)P$$

$$= P^{-1}(A - zI)P.$$

Remark

$$P^{-1}AP - zI = P^{-1}AP - zP^{-1}P$$

$$= P^{-1}AP - P^{-1}(zI)P$$

$$= P^{-1}(A - zI)P.$$

Therefore,

$$\det(\mathbf{A}-z\mathbf{I})=\det(\mathbf{P}^{-1}\mathbf{A}\mathbf{P}-z\mathbf{I}).$$

The Case of the Identity Matrix

The Case of the Identity Matrix

For $I_n \in \mathbb{R}^{n \times n}$,

- what is $p_{\mathbf{I}}(\lambda)$?
- What are its eigenvalues and the associated eigenvectors?
- What are the eigenspaces?

ullet $oldsymbol{A}$ and $oldsymbol{A}^ op$ possess the same eigenvalues

 A and A^T possess the same eigenvalues but not necessarily the same eigenvectors.

- ${\bf A}$ and ${\bf A}^{ op}$ possess the same eigenvalues but not necessarily the same eigenvectors.
- The eigenspace E_{λ} is null($\mathbf{A} \lambda \mathbf{I}$).

- A and A^T possess the same eigenvalues but not necessarily the same eigenvectors.
- The eigenspace E_{λ} is null($\mathbf{A} \lambda \mathbf{I}$).

$$\begin{aligned} \textbf{A}\textbf{x} &= \lambda \textbf{x} &\Leftrightarrow & \textbf{A}\textbf{x} - \lambda \textbf{x} &= \textbf{0} \\ &\Leftrightarrow & (\textbf{A} - \lambda \textbf{I})\textbf{x} &= \textbf{0} \\ &\Leftrightarrow & \textbf{x} \in \ker(\textbf{A} - \lambda \textbf{I}). \end{aligned}$$

- A and A^T possess the same eigenvalues but not necessarily the same eigenvectors.
- The eigenspace E_{λ} is null($\mathbf{A} \lambda \mathbf{I}$).

$$\begin{aligned} \mathbf{A}\mathbf{x} &= \lambda \mathbf{x} &\Leftrightarrow & \mathbf{A}\mathbf{x} - \lambda \mathbf{x} &= \mathbf{0} \\ &\Leftrightarrow & (\mathbf{A} - \lambda \mathbf{I})\mathbf{x} &= \mathbf{0} \\ &\Leftrightarrow & \mathbf{x} \in \ker(\mathbf{A} - \lambda \mathbf{I}). \end{aligned}$$

 Symmetric, positive definite matrices always have positive, real eigenvalues.

- A and A^T possess the same eigenvalues but not necessarily the same eigenvectors.
- The eigenspace E_{λ} is null($\mathbf{A} \lambda \mathbf{I}$).

$$\begin{aligned} \textbf{\textit{A}} \textbf{\textit{x}} &= \lambda \textbf{\textit{x}} & \Leftrightarrow & \textbf{\textit{A}} \textbf{\textit{x}} - \lambda \textbf{\textit{x}} = \textbf{\textit{0}} \\ & \Leftrightarrow & (\textbf{\textit{A}} - \lambda \textbf{\textit{I}}) \textbf{\textit{x}} = \textbf{\textit{0}} \\ & \Leftrightarrow & \textbf{\textit{x}} \in \ker(\textbf{\textit{A}} - \lambda \textbf{\textit{I}}). \end{aligned}$$

- Symmetric, positive definite matrices always have positive, real eigenvalues.
 - $\mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x} = \mathbf{x}^{\mathsf{T}} \lambda \mathbf{x}$



- A and A^T possess the same eigenvalues but not necessarily the same eigenvectors.
- The eigenspace E_{λ} is null($\mathbf{A} \lambda \mathbf{I}$).

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x} \Leftrightarrow \mathbf{A}\mathbf{x} - \lambda\mathbf{x} = \mathbf{0}$$

 $\Leftrightarrow (\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}$
 $\Leftrightarrow \mathbf{x} \in \ker(\mathbf{A} - \lambda\mathbf{I}).$

- Symmetric, positive definite matrices always have positive, real eigenvalues.
 - $\mathbf{x}^{\top} \mathbf{A} \mathbf{x} = \mathbf{x}^{\top} \lambda \mathbf{x} = \lambda \|\mathbf{x}\|^2 > 0.$

Theorem (4.13)

The eigenvectors $\mathbf{x}_1, \dots, \mathbf{x}_n$ of a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ with n distinct eigenvalues $\lambda_1, \dots, \lambda_n$ are linearly independent.

Theorem (4.14)

Given a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$, we can always obtain a symmetric, positive semidefinite matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$ by defining

$$\mathbf{S} := \mathbf{A}^{\top} \mathbf{A}$$
.

If rank(\boldsymbol{A}) = n, then $S := \boldsymbol{A}^{\top} \boldsymbol{A}$ is symmetric, positive definite.

◆ロト ◆団ト ◆豆ト ◆豆ト 豆 めので

Theorem

If ${m A}$ is symmetric, then eigenvectors to different eigenvalues are orthogonal.

Proof.

- Assume that $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ and $\mathbf{A}\mathbf{w} = \mu\mathbf{w}$ for two eigenvectors $\mathbf{v}, \mathbf{w} \in V$ corresponding to eigenvalues λ and μ such that $\lambda \neq \mu$.
- $\begin{array}{lll} ^{\bullet} & \lambda \langle \mathbf{v}, \mathbf{w} \rangle & = & \langle \lambda \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{A} \mathbf{v}, \mathbf{w} \rangle = (\mathbf{A} \mathbf{v})^{\top} \mathbf{w} = \mathbf{v}^{\top} \mathbf{A}^{\top} \mathbf{w} = \langle \mathbf{v}, \mathbf{A}^{\top} \mathbf{w} \rangle \\ & = & \langle \mathbf{v}, \mathbf{A} \mathbf{w} \rangle = \langle \mathbf{v}, \mu \mathbf{w} \rangle = \mu \langle \mathbf{v}, \mathbf{w} \rangle. \end{array}$

The equalities hold only if $\langle \mathbf{v}, \mathbf{w} \rangle = 0$.



Theorem (4.15; Spectral Theorem)

If $\mathbf{A} \in \mathbb{R}^{n \times n}$ is symmetric, then there exists an orthonormal basis, consisting of eigenvectors of \mathbf{A} , of the corresponding vector space V, and each eigenvalue is real.

Theorem (4.15; Spectral Theorem)

If $\mathbf{A} \in \mathbb{R}^{n \times n}$ is symmetric, then there exists an orthonormal basis, consisting of eigenvectors of \mathbf{A} , of the corresponding vector space V, and each eigenvalue is real.

Example

Consider

$$\mathbf{A} = \left[\begin{array}{rrr} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{array} \right]$$

Theorem (4.15; Spectral Theorem)

If $\mathbf{A} \in \mathbb{R}^{n \times n}$ is symmetric, then there exists an orthonormal basis, consisting of eigenvectors of \mathbf{A} , of the corresponding vector space V, and each eigenvalue is real.

Example

Consider

$$\mathbf{A} = \left[\begin{array}{rrr} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{array} \right]$$

Compute
$$p_{\mathbf{A}}(\lambda) = -(\lambda - 1)^2(\lambda - 7)$$

4 D > 4 D > 4 E > 4 E > E 990

Theorem (4.15; Spectral Theorem)

If $\mathbf{A} \in \mathbb{R}^{n \times n}$ is symmetric, then there exists an orthonormal basis, consisting of eigenvectors of \mathbf{A} , of the corresponding vector space V, and each eigenvalue is real.

Example

Consider

$$\mathbf{A} = \left[\begin{array}{rrr} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{array} \right]$$

Compute
$$p_{\mathbf{A}}(\lambda) = -(\lambda - 1)^2(\lambda - 7) \quad \Rightarrow \quad \lambda_1 = 1$$
 (repeated), $\lambda_2 = 7$.

10) 1A) 1 =) 1 =) 9 0 0

ML Math - Linear Algebra Eigenvalues & Eigenvectors

•
$$E_1 = \operatorname{span}(\mathbf{x}_1, \mathbf{x}_2)$$
, where $\mathbf{x}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$,

$$E_7 = \operatorname{span}(\mathbf{x}_3)$$
, where $\mathbf{x}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$.

22 / 47

Joseph C. C. Lin (CSE, NTOU, TW) ML Math - Linear Algebra Fall 2025

•
$$E_1 = \operatorname{span}(\mathbf{x}_1, \mathbf{x}_2)$$
, where $\mathbf{x}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$,

$$E_7 = \operatorname{span}(\mathbf{x}_3)$$
, where $\mathbf{x}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$.

• $\mathbf{x}_3 \perp \mathbf{x}_1, \mathbf{x}_2$ but $\mathbf{x}_1 \not\perp \mathbf{x}_2$.

Joseph C. C. Lin (CSE, NTOU, TW)

•
$$E_1 = \operatorname{span}(\mathbf{x}_1, \mathbf{x}_2)$$
, where $\mathbf{x}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$,

$$E_7 = \operatorname{span}(\mathbf{x}_3)$$
, where $\mathbf{x}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$.

- $\mathbf{x}_3 \perp \mathbf{x}_1, \mathbf{x}_2$ but $\mathbf{x}_1 \not\perp \mathbf{x}_2$.
- Note: Any linear combination of x₁ and x₂ is also an eigenvector of
 A w.r.t. λ₁.

•
$$E_1 = \operatorname{span}(\mathbf{x}_1, \mathbf{x}_2)$$
, where $\mathbf{x}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$, $\mathbf{x}_2 = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$,

$$E_7 = \operatorname{span}(\mathbf{x}_3)$$
, where $\mathbf{x}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$.

- $\mathbf{x}_3 \perp \mathbf{x}_1, \mathbf{x}_2$ but $\mathbf{x}_1 \not\perp \mathbf{x}_2$.
- Note: Any linear combination of x₁ and x₂ is also an eigenvector of Α w.r.t. λ₁.

$$\mathbf{A}(\alpha \mathbf{x}_1 + \beta \mathbf{x}_2) = \mathbf{A} \mathbf{x}_1 \alpha + \mathbf{A} \mathbf{x}_2 \beta = \lambda (\alpha \mathbf{x}_1 + \beta \mathbf{x}_2).$$

 Use Gram-Schmidt algorithm to construct an orthogonal basis for span(x₁, x₂)!

4D> 4A> 4E> 4E> E 990

ML Math - Linear Algebra Eigenvalues & Eigenvectors

Take
$$\mathbf{u}_1 = \mathbf{x}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$$
,

Joseph C. C. Lin (CSE, NTOU, TW)

ML Math - Linear Algebra Eigenvalues & Eigenvectors

Take
$$\mathbf{u}_1 = \mathbf{x}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$$
,

$$\mathbf{u}_2 = \mathbf{x}_2 - \frac{\mathbf{u}_1 \mathbf{u}_1^\top}{\|\mathbf{u}_1\|^2} \mathbf{x}_2 =$$

◆ロト ◆母 ト ◆ 恵 ト ◆ 恵 ・ 夕 ○ ○

Take
$$\mathbf{u}_1 = \mathbf{x}_1 = \begin{bmatrix} -1 \\ 1 \\ 0 \end{bmatrix}$$
,

$$\mathbf{u}_{2} = \mathbf{x}_{2} - \frac{\mathbf{u}_{1}\mathbf{u}_{1}^{\top}}{\|\mathbf{u}_{1}\|^{2}}\mathbf{x}_{2} = \begin{bmatrix} -1\\0\\1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 & -1 & 0\\-1 & 1 & 0\\0 & 0 & 0 \end{bmatrix}\begin{bmatrix} -1\\0\\1 \end{bmatrix}$$
$$= -\frac{1}{2}\begin{bmatrix} 1\\1\\-2 \end{bmatrix}.$$

A Practical Example

- Google uses the eigenvector corresponding to the maximal eigenvalue of a matrix **A** to determine the rank of a page for search.
 - The PageRank algorithm was developed at Stanford University by Larry Page and Sergey Brin in 1996.

A Practical Example

- Google uses the eigenvector corresponding to the maximal eigenvalue of a matrix A to determine the rank of a page for search.
 - The PageRank algorithm was developed at Stanford University by Larry Page and Sergey Brin in 1996.
- Websites are represented as a huge directed graph (pages: vertices; links: edges).
- Compute the weight (importance) $x_i \ge 0$ for a website a_i and get \mathbf{x} .
 - The number of pages pointing to a_i .
- A transition matrix **A** (prob.): modeling the navigation behavior of a user.
- Goal: x, Ax, A²x, ..., x*

A Practical Example

- Google uses the eigenvector corresponding to the maximal eigenvalue of a matrix **A** to determine the rank of a page for search.
 - The PageRank algorithm was developed at Stanford University by Larry Page and Sergey Brin in 1996.
- Websites are represented as a huge directed graph (pages: vertices; links: edges).
- Compute the weight (importance) $x_i \ge 0$ for a website a_i and get \mathbf{x} .
 - The number of pages pointing to a_i .
- A transition matrix **A** (prob.): modeling the navigation behavior of a user.
- Goal: \mathbf{x} , $\mathbf{A}\mathbf{x}$, $\mathbf{A}^2\mathbf{x}$, ..., \mathbf{x}^* \Rightarrow $\mathbf{A}\mathbf{x}^* = \mathbf{x}^*$ \Rightarrow Turning to probabilities (normalization).

◆ロト→□ト→ミト→ミト ミ りの

Outline

- 1 Eigenvalues & Eigenvectors
- Cholesky Decomposition
- 3 Eigendecomposition & Diagonalization

Cholesky Decomposition

Cholesky Decomposition

A symmetric, positive definite matrix \mathbf{A} can be factorized into a product $\mathbf{A} = \mathbf{L} \mathbf{L}^{\top}$, where \mathbf{L} is a lower-triangular matrix with positive diagonal elements.

Example of Cholesky Factorization

$$\boldsymbol{A} = \left[\begin{array}{ccc} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{array} \right] = \boldsymbol{L} \boldsymbol{L}^{\top} = \left[\begin{array}{ccc} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{array} \right] \left[\begin{array}{ccc} \ell_{11} & \ell_{21} & \ell_{31} \\ 0 & \ell_{22} & \ell_{32} \\ 0 & 0 & \ell_{33} \end{array} \right].$$

We have

$$\textbf{\textit{A}} = \left[\begin{array}{ccc} \ell_{11}^2 & \ell_{21}\ell_{11} & \ell_{31}\ell_{11} \\ \ell_{21}\ell_{11} & \ell_{21}^2 + \ell_{22}^2 & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} \\ \ell_{31}\ell_{11} & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{array} \right]$$

Finally, solve $\ell_{11}, \ldots, \ell_{33}$.

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \ell_{11}^2 & \ell_{21}\ell_{11} & \ell_{31}\ell_{11} \\ \ell_{21}\ell_{11} & \ell_{21}^2 + \ell_{22}^2 & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} \\ \ell_{31}\ell_{11} & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{bmatrix}$$

•
$$\ell_{11} = \sqrt{a_{11}}$$
,

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \ell_{11}^2 & \ell_{21}\ell_{11} & \ell_{31}\ell_{11} \\ \ell_{21}\ell_{11} & \ell_{21}^2 + \ell_{22}^2 & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} \\ \ell_{31}\ell_{11} & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{bmatrix}$$

$$\bullet \ \ell_{11} = \sqrt{a_{11}}, \quad \ell_{21} = \frac{a_{21}}{\ell_{11}},$$

<ロト 4回 ト 4 直 ト 4 直 ト 直 り 9 (で

$$\mathbf{A} = \left[\begin{array}{ccc} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{array} \right] = \left[\begin{array}{ccc} \ell_{11}^2 & \ell_{21}\ell_{11} & \ell_{31}\ell_{11} \\ \ell_{21}\ell_{11} & \ell_{21}^2 + \ell_{22}^2 & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} \\ \ell_{31}\ell_{11} & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{array} \right]$$

•
$$\ell_{11} = \sqrt{a_{11}}$$
, $\ell_{21} = \frac{a_{21}}{\ell_{11}}$, $\ell_{22} = \sqrt{a_{22} - \ell_{21}^2}$,

•
$$\ell_{11} = \sqrt{a_{11}}$$
, $\ell_{21} = \frac{a_{21}}{\ell_{11}}$, $\ell_{22} = \sqrt{a_{22} - \ell_{21}^2}$, $\ell_{31} = \frac{a_{31}}{\ell_{11}}$, $\ell_{32} = \frac{a_{32} - \ell_{31}\ell_{21}}{\ell_{22}}$,

$$\mathbf{A} = \left[\begin{array}{ccc} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{array} \right] = \left[\begin{array}{ccc} \ell_{11}^2 & \ell_{21}\ell_{11} & \ell_{31}\ell_{11} \\ \ell_{21}\ell_{11} & \ell_{21}^2 + \ell_{22}^2 & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} \\ \ell_{31}\ell_{11} & \ell_{31}\ell_{21} + \ell_{32}\ell_{22} & \ell_{31}^2 + \ell_{32}^2 + \ell_{33}^2 \end{array} \right]$$

•
$$\ell_{11} = \sqrt{a_{11}}$$
, $\ell_{21} = \frac{a_{21}}{\ell_{11}}$, $\ell_{22} = \sqrt{a_{22} - \ell_{21}^2}$, $\ell_{31} = \frac{a_{31}}{\ell_{11}}$, $\ell_{32} = \frac{a_{32} - \ell_{31}\ell_{21}}{\ell_{22}}$, $\ell_{33} = \sqrt{a_{33} - \ell_{31}^2 - \ell_{32}^2}$.

Motivations of Using Cholesky Decomposition

- Symmetric positive definite matrices require frequent manipulation.
 - E.g., Covariance matrix of a multivariate Gaussian variable.
 - The Cholesky factorization of the covariance matrix allows us to generate samples from a Gaussian distribution.
- Computing gradients in deep stochastic models such as variational auto-encoder (VAE).

Motivations of Using Cholesky Decomposition

- Symmetric positive definite matrices require frequent manipulation.
 - E.g., Covariance matrix of a multivariate Gaussian variable.
 - The Cholesky factorization of the covariance matrix allows us to generate samples from a Gaussian distribution.
- Computing gradients in deep stochastic models such as variational auto-encoder (VAE).
- Compute determinants efficiently.
 - $\det(\mathbf{A}) = \det(\mathbf{L}) \det(\mathbf{L}^{\top}) = \det(\mathbf{L})^2$.
 - Note: det(L) can be computed efficiently (: triangular).

Outline

1 Eigenvalues & Eigenvectors

- 2 Cholesky Decomposition
- 3 Eigendecomposition & Diagonalization

 Diagonalization is an important application of basis change and eigenvalues.

- Diagonalization is an important application of basis change and eigenvalues.
- Diagonalization allow fast computation of determinants, powers and inverses of matrices.

- Diagonalization is an important application of basis change and eigenvalues.
- Diagonalization allow fast computation of determinants, powers and inverses of matrices. A diagonal matrix is like

$$\mathbf{D} = \left[\begin{array}{ccc} c_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & c_n \end{array} \right].$$

- Diagonalization is an important application of basis change and eigenvalues.
- Diagonalization allow fast computation of determinants, powers and inverses of matrices. A diagonal matrix is like

$$\mathbf{D} = \left[\begin{array}{ccc} c_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & c_n \end{array} \right].$$

• Question: What are the determinant, cubic, and inverse of D?

Similarity

Similarity

Two matrices A and $B \in \mathbb{R}^{n \times n}$ are similar if there exists an invertible matrix $S \in \mathbb{R}^{n \times n}$ such that $A = S^{-1}BS$.

Similarity

Similarity

Two matrices \boldsymbol{A} and $\boldsymbol{B} \in \mathbb{R}^{n \times n}$ are similar if there exists an invertible matrix $\boldsymbol{S} \in \mathbb{R}^{n \times n}$ such that $\boldsymbol{A} = \boldsymbol{S}^{-1} \boldsymbol{B} \boldsymbol{S}$.

Diagonalizable

A matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is diagonalizable if it is *similar* to a *diagonal* matrix..

Similarity

Similarity

Two matrices \boldsymbol{A} and $\boldsymbol{B} \in \mathbb{R}^{n \times n}$ are similar if there exists an invertible matrix $\boldsymbol{S} \in \mathbb{R}^{n \times n}$ such that $\boldsymbol{A} = \boldsymbol{S}^{-1} \boldsymbol{B} \boldsymbol{S}$.

Diagonalizable

A matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is diagonalizable if it is similar to a diagonal matrix...

• $\exists \mathbf{D} \in \mathbb{R}^{n \times n}$, such that $\mathbf{D} = \mathbf{P}^{-1} \mathbf{A} \mathbf{P}$.

Eigenvectors & Diagonalization

- Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ and $\lambda_1, \dots, \lambda_n$ be a set of scalars.
- Let $\mathbf{p}_1, \dots, \mathbf{p}_n$ be a set of vectors in \mathbb{R}^n .
- Let $\mathbf{D} \in \mathbb{R}^{n \times n}$ be a diagonal matrix with diagonal entries $\lambda_1, \dots, \lambda_n$.

We can show that

$$AP = PD$$
.

if and only if $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of \boldsymbol{A} and $\mathbf{p}_1, \ldots, \mathbf{p}_n$ are the corresponding eigenvectors of \boldsymbol{A} .

We can see that

$$AP = A[p_1, \dots, p_n] = [Ap_1, \dots, Ap_n],$$

and

We can see that

$$AP = A[p_1, \dots, p_n] = [Ap_1, \dots, Ap_n],$$

and

$$PD = [\mathbf{p}_1, \dots, \mathbf{p}_n] \begin{bmatrix} \lambda_1 & 0 \\ & \ddots & \\ 0 & \lambda_n \end{bmatrix}$$

We can see that

$$AP = A[p_1, \dots, p_n] = [Ap_1, \dots, Ap_n],$$

and

$$PD = [\mathbf{p}_1, \dots, \mathbf{p}_n] \begin{bmatrix} \lambda_1 & 0 \\ & \ddots \\ 0 & \lambda_n \end{bmatrix} = [\lambda_1 \mathbf{p}_1, \dots, \lambda_n \mathbf{p}_n].$$

We can see that

$$\textbf{\textit{AP}} = \textbf{\textit{A}}[\textbf{\textit{p}}_1, \dots, \textbf{\textit{p}}_n] = [\textbf{\textit{A}}\textbf{\textit{p}}_1, \dots, \textbf{\textit{A}}\textbf{\textit{p}}_n],$$

and

$$PD = [\mathbf{p}_1, \dots, \mathbf{p}_n] \begin{bmatrix} \lambda_1 & 0 \\ & \ddots \\ 0 & \lambda_n \end{bmatrix} = [\lambda_1 \mathbf{p}_1, \dots, \lambda_n \mathbf{p}_n].$$

Thus,

$$\mathbf{A}\mathbf{p}_1 = \lambda_1\mathbf{p}_1$$
 \vdots
 $\mathbf{A}\mathbf{p}_n = \lambda_n\mathbf{p}_n$

Therefore, the columns of P are eigenvectors of A.

• If n=1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.

- If n = 1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.
- Assume that $\mathbf{p}_1, \dots, \mathbf{p}_{n-1}$ are linearly independent.

- If n=1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.
- Assume that $\mathbf{p}_1, \dots, \mathbf{p}_{n-1}$ are linearly independent.
- Suppose that $\alpha_1 \mathbf{p}_1 + \alpha_2 \mathbf{p}_2 + \cdots + \alpha_n \mathbf{p}_n = \mathbf{0}$. (*)

- If n=1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.
- Assume that $\mathbf{p}_1, \dots, \mathbf{p}_{n-1}$ are linearly independent.
- Suppose that $\alpha_1 \mathbf{p}_1 + \alpha_2 \mathbf{p}_2 + \cdots + \alpha_n \mathbf{p}_n = \mathbf{0}$. (*)
- \Rightarrow $\mathbf{A}(\alpha_1\mathbf{p}_1 + \alpha_2\mathbf{p}_2 + \cdots + \alpha_n\mathbf{p}_n) = \mathbf{A0} = \mathbf{0}.$

- If n=1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.
- Assume that $\mathbf{p}_1, \dots, \mathbf{p}_{n-1}$ are linearly independent.
- Suppose that $\alpha_1 \mathbf{p}_1 + \alpha_2 \mathbf{p}_2 + \cdots + \alpha_n \mathbf{p}_n = \mathbf{0}$. (*)
- \Rightarrow $\mathbf{A}(\alpha_1\mathbf{p}_1 + \alpha_2\mathbf{p}_2 + \cdots + \alpha_n\mathbf{p}_n) = \mathbf{A0} = \mathbf{0}.$
- $\Rightarrow \alpha \lambda_1 \mathbf{p}_1 + \alpha_2 \lambda_2 \mathbf{p}_2 + \dots + \alpha_n \lambda_n \mathbf{p}_n = \mathbf{0}. \quad (**)$
- $\Rightarrow (**) \lambda_n \cdot (*):$ $\alpha_1(\lambda_1 \lambda_n)\mathbf{p}_1 + \alpha_2(\lambda_2 \lambda_n)\mathbf{p}_2 + \dots + \alpha_{n-1}(\lambda_{n-1} \lambda_n)\mathbf{p}_{n-1} = \mathbf{0}.$

- If n=1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.
- Assume that p_1, \ldots, p_{n-1} are linearly independent.
- Suppose that $\alpha_1 \mathbf{p}_1 + \alpha_2 \mathbf{p}_2 + \cdots + \alpha_n \mathbf{p}_n = \mathbf{0}$. (*)
- \Rightarrow $\mathbf{A}(\alpha_1\mathbf{p}_1 + \alpha_2\mathbf{p}_2 + \cdots + \alpha_n\mathbf{p}_n) = \mathbf{A0} = \mathbf{0}.$
- $\Rightarrow \alpha \lambda_1 \mathbf{p}_1 + \alpha_2 \lambda_2 \mathbf{p}_2 + \dots + \alpha_n \lambda_n \mathbf{p}_n = \mathbf{0}. \quad (**)$
- \Rightarrow (**) $-\lambda_n \cdot (*)$:

$$\alpha_1(\lambda_1-\lambda_n)\mathbf{p}_1+\alpha_2(\lambda_2-\lambda_n)\mathbf{p}_2+\cdots+\alpha_{n-1}(\lambda_{n-1}-\lambda_n)\mathbf{p}_{n-1}=\mathbf{0}.$$

- $\Rightarrow \alpha_i(\lambda_1 \lambda_n) = 0$ for each i = 1, 2, ..., n 1.
- $\Rightarrow \alpha_i = 0$ for each $i = 1, 2, \dots, n-1$.

- If n=1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.
- Assume that $\mathbf{p}_1, \dots, \mathbf{p}_{n-1}$ are linearly independent.
- Suppose that $\alpha_1 \mathbf{p}_1 + \alpha_2 \mathbf{p}_2 + \cdots + \alpha_n \mathbf{p}_n = \mathbf{0}$. (*)
- \Rightarrow $\mathbf{A}(\alpha_1\mathbf{p}_1 + \alpha_2\mathbf{p}_2 + \cdots + \alpha_n\mathbf{p}_n) = \mathbf{A0} = \mathbf{0}.$
- $\Rightarrow \alpha \lambda_1 \mathbf{p}_1 + \alpha_2 \lambda_2 \mathbf{p}_2 + \dots + \alpha_n \lambda_n \mathbf{p}_n = \mathbf{0}. \quad (**)$
- \Rightarrow (**) $-\lambda_n \cdot (*)$:

$$\alpha_1(\lambda_1-\lambda_n)\mathbf{p}_1+\alpha_2(\lambda_2-\lambda_n)\mathbf{p}_2+\cdots+\alpha_{n-1}(\lambda_{n-1}-\lambda_n)\mathbf{p}_{n-1}=\mathbf{0}.$$

- $\Rightarrow \alpha_i(\lambda_1 \lambda_n) = 0$ for each i = 1, 2, ..., n 1.
- $\Rightarrow \alpha_i = 0$ for each $i = 1, 2, ..., n 1. \Rightarrow \alpha_n = 0$.

- If n=1, we only get $\mathbf{p}_1 \ (\neq \mathbf{0}) \Rightarrow$ linearly independent.
- Assume that $\mathbf{p}_1, \dots, \mathbf{p}_{n-1}$ are linearly independent.
- Suppose that $\alpha_1 \mathbf{p}_1 + \alpha_2 \mathbf{p}_2 + \cdots + \alpha_n \mathbf{p}_n = \mathbf{0}$. (*)
- \Rightarrow $\mathbf{A}(\alpha_1\mathbf{p}_1 + \alpha_2\mathbf{p}_2 + \cdots + \alpha_n\mathbf{p}_n) = \mathbf{A0} = \mathbf{0}.$
- $\Rightarrow \alpha \lambda_1 \mathbf{p}_1 + \alpha_2 \lambda_2 \mathbf{p}_2 + \dots + \alpha_n \lambda_n \mathbf{p}_n = \mathbf{0}. \quad (**)$
- \Rightarrow (**) $-\lambda_n \cdot$ (*):

$$\alpha_1(\lambda_1-\lambda_n)\mathbf{p}_1+\alpha_2(\lambda_2-\lambda_n)\mathbf{p}_2+\cdots+\alpha_{n-1}(\lambda_{n-1}-\lambda_n)\mathbf{p}_{n-1}=\mathbf{0}.$$

- $\Rightarrow \alpha_i(\lambda_1 \lambda_n) = 0$ for each i = 1, 2, ..., n 1.
- $\Rightarrow \alpha_i = 0$ for each i = 1, 2, ..., n 1. $\Rightarrow \alpha_n = 0$.
 - $\bullet :: \alpha_1 = \alpha_2 = \cdots = \alpha_n = 0.$

◆ロト ◆団 ト ◆ 豆 ト ◆ 豆 ・ 夕 Q (~)

Eigendecomposition (Diagonalization)

${\sf Theorem}$ [Eigendecomposition (Diagonalization)]

A square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ can be factored into

$$\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1},$$

where $P \in \mathbb{R}^{n \times n}$ and D is a diagonal matrix whose diagonal entries are the eigenvalues of A

if and only if

the eigenvectors of \mathbf{A} form a basis of \mathbb{R}^n .

Put it concisely

Theorem

For a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, the following statements are equivalent:

- A is diagonalizable.
- **A** has *n* linearly independent eigenvectors.

Remark

The spectral theorem tells us that:

We can find an orthonormal basis of the corresponding vector space consisting of eigenvectors of of a symmetric matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$

Remark

The spectral theorem tells us that:

We can find an orthonormal basis of the corresponding vector space consisting of eigenvectors of of a symmetric matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$.

Theorem

A symmetric matrix $\mathbf{S} \in \mathbb{R}^{n \times n}$ can be always diagonalized.

Compute the eigendecomposition of
$$\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$$
.

Compute the eigenvalues and eigenvectors.

Compute the eigendecomposition of
$$\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$$
.

Compute the eigenvalues and eigenvectors.

$$\det(\mathbf{A} - \lambda \mathbf{I}) = \det\left(\begin{bmatrix} \frac{5}{2} - \lambda & -1 \\ -1 & \frac{5}{2} - \lambda \end{bmatrix} \right) =$$

Compute the eigendecomposition of
$$\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$$
.

Compute the eigenvalues and eigenvectors.

$$\det(\mathbf{A} - \lambda \mathbf{I}) = \det\left(\left[\begin{array}{cc} \frac{5}{2} - \lambda & -1 \\ -1 & \frac{5}{2} - \lambda \end{array} \right] \right) = \left(\lambda - \frac{7}{2} \right) \left(\lambda - \frac{3}{2} \right).$$

Set
$$\lambda_1 = \frac{7}{2}, \lambda_2 = \frac{3}{2}$$
.

2 Solving $\mathbf{A}\mathbf{p}_1 = \frac{7}{2}\mathbf{p}_1$ and $\mathbf{A}\mathbf{p}_2 = \frac{3}{2}\mathbf{p}_2$.

Compute the eigendecomposition of
$$\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$$
.

Compute the eigenvalues and eigenvectors.

$$\det(\textbf{\textit{A}}-\lambda\textbf{\textit{I}}) = \det\left(\left[\begin{array}{cc} \frac{5}{2}-\lambda & -1 \\ -1 & \frac{5}{2}-\lambda \end{array}\right]\right) = \left(\lambda - \frac{7}{2}\right)\left(\lambda - \frac{3}{2}\right).$$

Set
$$\lambda_1 = \frac{7}{2}, \lambda_2 = \frac{3}{2}$$
.

② Solving $\mathbf{A}\mathbf{p}_1 = \frac{7}{2}\mathbf{p}_1$ and $\mathbf{A}\mathbf{p}_2 = \frac{3}{2}\mathbf{p}_2$.

$$\textbf{p}_1 = \frac{1}{\sqrt{2}} \left[\begin{array}{c} 1 \\ -1 \end{array} \right], \ \ \textbf{p}_2 = \frac{1}{\sqrt{2}} \left[\begin{array}{c} 1 \\ 1 \end{array} \right].$$

Compute the eigendecomposition of
$$\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$$
.

$$\mathbf{p}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad \mathbf{p}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

3 Check for independency of $\{\mathbf{p}_1, \mathbf{p}_2\}$. \Longrightarrow

Compute the eigendecomposition of $\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$.

$$\mathbf{p}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad \mathbf{p}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

- **3** Check for independency of $\{\mathbf{p}_1, \mathbf{p}_2\}$. $\Longrightarrow \checkmark$
- Construct P:

Compute the eigendecomposition of
$$\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$$
.

$$\mathbf{p}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \ \mathbf{p}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

- $\textbf{ § Check for independency of } \{\textbf{p}_1,\textbf{p}_2\}. \Longrightarrow \checkmark$
- **3** Construct $P: \Longrightarrow P = [\mathbf{p}_1, \ \mathbf{p}_2] = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$.
 - \star Note that $\{\mathbf{p}_1, \mathbf{p}_2\}$ forms an orthonormal basis

Compute the eigendecomposition of $\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$.

$$\mathbf{p}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad \mathbf{p}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

- $\textbf{ § Check for independency of } \{\textbf{p}_1,\textbf{p}_2\}. \Longrightarrow \checkmark$
- **3** Construct $P: \Longrightarrow P = [\mathbf{p}_1, \ \mathbf{p}_2] = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$.
 - * Note that $\{\mathbf{p}_1, \mathbf{p}_2\}$ forms an orthonormal basis $\mathbf{P}^{-1} = \mathbf{P}^{\top}$. (Exercise)

Compute the eigendecomposition of $\mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$.

$$\mathbf{p}_1 = rac{1}{\sqrt{2}} \left[egin{array}{c} 1 \\ -1 \end{array}
ight], \ \mathbf{p}_2 = rac{1}{\sqrt{2}} \left[egin{array}{c} 1 \\ 1 \end{array}
ight].$$

- $\textbf{ § Check for independency of } \{\textbf{p}_1,\textbf{p}_2\}. \Longrightarrow \checkmark$
- Construct $P: \Longrightarrow P = [\mathbf{p}_1, \ \mathbf{p}_2] = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$.
 - * Note that $\{\mathbf{p}_1, \mathbf{p}_2\}$ forms an orthonormal basis $\mathbf{P}^{-1} = \mathbf{P}^{\top}$. (Exercise)

Finally we obtain $\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1}$.

<ロ > ← □ > ← □ > ← □ > ← □ ● ● の へ ○

•
$$A^k = (PDP^{-1})^k$$

•
$$A^k = (PDP^{-1})^k = (PDP^{-1})(PDP^{-1})\cdots(PDP^{-1})$$

•
$$A^k = (PDP^{-1})^k = (PDP^{-1})(PDP^{-1})\cdots(PDP^{-1}) = PD^kP^{-1}$$
.

•
$$\mathbf{A}^k = (PDP^{-1})^k = (PDP^{-1})(PDP^{-1}) \cdots (PDP^{-1}) = PD^kP^{-1}$$
.

$$\bullet \ \det(\mathbf{A}) = \det(\mathbf{P}\mathbf{D}\mathbf{P}^{-1})$$

•
$$A^k = (PDP^{-1})^k = (PDP^{-1})(PDP^{-1})\cdots(PDP^{-1}) = PD^kP^{-1}$$
.

$$\bullet \ \det(\mathbf{A}) = \det(\mathbf{P}\mathbf{D}\mathbf{P}^{-1}) = \det(\mathbf{P})\det(\mathbf{D})\det(\mathbf{P}^{-1})$$

•
$$A^k = (PDP^{-1})^k = (PDP^{-1})(PDP^{-1}) \cdots (PDP^{-1}) = PD^kP^{-1}$$
.

•
$$\det(\mathbf{A}) = \det(\mathbf{P}\mathbf{D}\mathbf{P}^{-1}) = \det(\mathbf{P})\det(\mathbf{D})\det(\mathbf{P}^{-1}) = \det(\mathbf{D}) = \prod_i d_{ii}$$
.

Another Application: Using Maclaurin Series

Maclaurin Series

A Maclaurin Series expansion of f(x) is

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f^{(3)}(0)}{3!}x^3 + \dots + \frac{f^{(n)}(0)}{n!}x^n + \dots$$

Another Application: Using Maclaurin Series

Maclaurin Series

A Maclaurin Series expansion of f(x) is

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f^{(3)}(0)}{3!}x^3 + \dots + \frac{f^{(n)}(0)}{n!}x^n + \dots$$

For example, suppose $f(x) = e^x$, then

$$f(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

Another Application: Using Maclaurin Series

Maclaurin Series

A Maclaurin Series expansion of f(x) is

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f^{(3)}(0)}{3!}x^3 + \dots + \frac{f^{(n)}(0)}{n!}x^n + \dots$$

For example, suppose $f(x) = e^x$, then

$$f(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots$$

Thus, for $\mathbf{A} \in \mathbb{R}^{n \times n}$ such that $\mathbf{A} = \mathbf{P} \mathbf{D} \mathbf{P}^{-1}$, we may define

$$f(\mathbf{A}) = \mathbf{P}f(\mathbf{D})\mathbf{P}^{-1}.$$

◆□ → ◆□ → ◆ ■ → ■ り へ ○

Another Application: Using Maclaurin Series

Maclaurin Series

A Maclaurin Series expansion of f(x) is

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f^{(3)}(0)}{3!}x^3 + \dots + \frac{f^{(n)}(0)}{n!}x^n + \dots$$

For example, suppose $f(\mathbf{A}) = e^{\mathbf{A}}$, then

$$f(\mathbf{A}) = \mathbf{I} + \mathbf{A} + \frac{\mathbf{A}^2}{2!} + \frac{\mathbf{A}^3}{3!} + \cdots$$

Another Application: Using Maclaurin Series

Maclaurin Series

A Maclaurin Series expansion of f(x) is

$$f(x) = f(0) + f'(0)x + \frac{f''(0)}{2!}x^2 + \frac{f^{(3)}(0)}{3!}x^3 + \dots + \frac{f^{(n)}(0)}{n!}x^n + \dots$$

For example, suppose $f(\mathbf{A}) = e^{\mathbf{A}}$, then

$$f(\mathbf{A}) = \mathbf{I} + \mathbf{A} + \frac{\mathbf{A}^2}{2!} + \frac{\mathbf{A}^3}{3!} + \cdots$$

Thus, for $\mathbf{A} \in \mathbb{R}^{n \times n}$ such that $\mathbf{A} = \mathbf{PDP}^{-1}$, we may define

$$e^{\mathbf{A}} = \mathbf{P}e^{\mathbf{D}}\mathbf{P}^{-1}.$$

←□ → ←□ → ← □ → □ → ○○○

$$e^{\pmb{A}} = \pmb{I} + \pmb{A} + \frac{\pmb{A}^2}{2!} + \frac{\pmb{A}^3}{3!} + \cdots$$

4 D > 4 D > 4 E > 4 E > E 990

Joseph C. C. Lin (CSE, NTOU, TW) ML Math - Linear Algebra Fall 2025 44 / 47

Indeed.

$$e^{\mathbf{A}} = \mathbf{I} + \mathbf{A} + \frac{\mathbf{A}^2}{2!} + \frac{\mathbf{A}^3}{3!} + \cdots$$

= $\mathbf{P}\mathbf{I}\mathbf{P}^{-1} + \mathbf{P}\mathbf{D}\mathbf{P}^{-1} + \frac{\mathbf{P}\mathbf{D}^2\mathbf{P}^{-1}}{2!} + \frac{\mathbf{P}\mathbf{D}^3\mathbf{P}^{-1}}{3!} + \cdots$

Joseph C. C. Lin (CSE, NTOU, TW) ML Math - Linear Algebra 44 / 47

$$e^{A} = I + A + \frac{A^{2}}{2!} + \frac{A^{3}}{3!} + \cdots$$

$$= PIP^{-1} + PDP^{-1} + \frac{PD^{2}P^{-1}}{2!} + \frac{PD^{3}P^{-1}}{3!} + \cdots$$

$$= P\left(I + D + \frac{D^{2}}{2!} + \frac{D^{3}}{3!} + \cdots\right)P^{-1}$$

Joseph C. C. Lin (CSE, NTOU, TW) ML Math - Linear Algebra

$$e^{\mathbf{A}} = \mathbf{I} + \mathbf{A} + \frac{\mathbf{A}^{2}}{2!} + \frac{\mathbf{A}^{3}}{3!} + \cdots$$

$$= \mathbf{P}\mathbf{I}\mathbf{P}^{-1} + \mathbf{P}\mathbf{D}\mathbf{P}^{-1} + \frac{\mathbf{P}\mathbf{D}^{2}\mathbf{P}^{-1}}{2!} + \frac{\mathbf{P}\mathbf{D}^{3}\mathbf{P}^{-1}}{3!} + \cdots$$

$$= \mathbf{P}\left(\mathbf{I} + \mathbf{D} + \frac{\mathbf{D}^{2}}{2!} + \frac{\mathbf{D}^{3}}{3!} + \cdots\right)\mathbf{P}^{-1}$$

$$= \mathbf{P}e^{\mathbf{D}}\mathbf{P}^{-1}$$

Joseph C. C. Lin (CSE, NTOU, TW)

$$e^{\mathbf{A}} = \mathbf{I} + \mathbf{A} + \frac{\mathbf{A}^{2}}{2!} + \frac{\mathbf{A}^{3}}{3!} + \cdots$$

$$= \mathbf{P}\mathbf{I}\mathbf{P}^{-1} + \mathbf{P}\mathbf{D}\mathbf{P}^{-1} + \frac{\mathbf{P}\mathbf{D}^{2}\mathbf{P}^{-1}}{2!} + \frac{\mathbf{P}\mathbf{D}^{3}\mathbf{P}^{-1}}{3!} + \cdots$$

$$= \mathbf{P}\left(\mathbf{I} + \mathbf{D} + \frac{\mathbf{D}^{2}}{2!} + \frac{\mathbf{D}^{3}}{3!} + \cdots\right)\mathbf{P}^{-1}$$

$$= \mathbf{P}e^{\mathbf{D}}\mathbf{P}^{-1}$$

Note that if
$$\mathbf{D} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$$
, we have $\mathbf{I} + \mathbf{D} + \frac{\mathbf{D}^2}{2!} + \frac{\mathbf{D}^3}{3!} + \cdots$

$$= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} + \frac{1}{2!} \begin{bmatrix} \lambda_1^2 & 0 \\ 0 & \lambda_2^2 \end{bmatrix} + \frac{1}{3!} \begin{bmatrix} \lambda_1^3 & 0 \\ 0 & \lambda_2^3 \end{bmatrix} + \cdots$$

$$= \begin{bmatrix} e^{\lambda_1} & 0 \\ 0 & e^{\lambda_2} \end{bmatrix}$$

◆□ → ◆□ → ◆ □ → ○ □ → ○ ○ ○

Compute
$$e^{\mathbf{A}}$$
 for $\mathbf{A} = \begin{bmatrix} -2 & -6 \\ 1 & 3 \end{bmatrix}$.

• Eigenvalues: 0, 1.

Compute
$$e^{\mathbf{A}}$$
 for $\mathbf{A} = \begin{bmatrix} -2 & -6 \\ 1 & 3 \end{bmatrix}$.

- Eigenvalues: 0, 1.
- Corresponding eigenvectors: $[-3 \ 1]^{\top}$, $[-2 \ 1]^{\top}$.

Compute
$$e^{\mathbf{A}}$$
 for $\mathbf{A} = \begin{bmatrix} -2 & -6 \\ 1 & 3 \end{bmatrix}$.

- Eigenvalues: 0, 1.
- Corresponding eigenvectors: $[-3 \ 1]^{\top}$, $[-2 \ 1]^{\top}$.

• Take
$$\mathbf{P} = \begin{bmatrix} -3 & -2 \\ 1 & 1 \end{bmatrix}$$
, and we have $\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{D} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$.

Compute
$$e^{\mathbf{A}}$$
 for $\mathbf{A} = \begin{bmatrix} -2 & -6 \\ 1 & 3 \end{bmatrix}$.

- Eigenvalues: 0, 1.
- Corresponding eigenvectors: $[-3 \ 1]^{\top}$, $[-2 \ 1]^{\top}$.
- Take $\mathbf{P} = \begin{bmatrix} -3 & -2 \\ 1 & 1 \end{bmatrix}$, and we have $\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{D} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$.
- Thus, $e^{\mathbf{A}} = \mathbf{P}f(\mathbf{D})\mathbf{P}^{-1}$, and note that

$$f(\mathbf{D}) =$$

Compute
$$e^{\mathbf{A}}$$
 for $\mathbf{A} = \begin{bmatrix} -2 & -6 \\ 1 & 3 \end{bmatrix}$.

- Eigenvalues: 0, 1.
- Corresponding eigenvectors: $[-3 \ 1]^{\top}$, $[-2 \ 1]^{\top}$.
- Take $\mathbf{P} = \begin{bmatrix} -3 & -2 \\ 1 & 1 \end{bmatrix}$, and we have $\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{D} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$.
- Thus, $e^{\mathbf{A}} = \mathbf{P}f(\mathbf{D})\mathbf{P}^{-1}$, and note that

$$f(\mathbf{D}) = \left[\begin{array}{cc} f(0) & 0 \\ 0 & f(1) \end{array} \right]$$

Compute
$$e^{\mathbf{A}}$$
 for $\mathbf{A} = \begin{bmatrix} -2 & -6 \\ 1 & 3 \end{bmatrix}$.

- Eigenvalues: 0, 1.
- Corresponding eigenvectors: $[-3 \ 1]^{\top}$, $[-2 \ 1]^{\top}$.
- Take $\mathbf{P} = \begin{bmatrix} -3 & -2 \\ 1 & 1 \end{bmatrix}$, and we have $\mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \mathbf{D} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$.
- Thus, $e^{\mathbf{A}} = \mathbf{P}f(\mathbf{D})\mathbf{P}^{-1}$, and note that

$$f(\mathbf{D}) = \begin{bmatrix} f(0) & 0 \\ 0 & f(1) \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & e \end{bmatrix}.$$

◆□▶◆□▶◆臺▶◆臺▶ 臺 かぐで

Remarks

- A square matrix can have a zero eigenvalue, but never has zero eigenvectors.
- A zero matrix **O** is diagonalizable, too.
 - All nonzero vectors are eigenvectors since all vectors ${\bf v}$ satisfy ${\bf O}{\bf v}=0{\bf v}.$

Discussions