Mathematics for Machine Learning
— Linear Algebra: Eigenvalues, Eigenvectors, Eigenspaces, Cholesky
Decomposition & Diagonalization

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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*

- Matrix decomposition or matrix factorization.

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- Three matrix decompositions will be introduced.

Outline

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1. Eigenvalues & Eigenvectors

2. Cholesky Decomposition

3. Eigendecomposition & Diagonalization

Characteristic Polynomial

Characteristic Polynomial

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

$$
\begin{aligned}
p_{\boldsymbol{A}}(\lambda) &:= \det(\boldsymbol{A} - \lambda \boldsymbol{I}) \\
&= (-1)^n (\lambda - \lambda_1) \cdots (\lambda - \lambda_n) \\
&= c_0 + c_1 \lambda + \cdots + c_{n-1} \lambda^{n-1} + (-1)^n \lambda^n,
\end{aligned}
$$

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

Note that

- $c_0 = \det(\boldsymbol{A})$

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- $c_{n-1} = (-1)^{n-1} \operatorname{tr}(\boldsymbol{A})$

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back

Example

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

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

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Given $\boldsymbol{B} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 4 & -17 & 8 \end{bmatrix}$,

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

Eigenvalue Equation

Eigenvalues & Eigenvectors

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

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

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

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

Equivalent statements:

- λ is an eigenvalue of $\boldsymbol{A} \in \mathbb{R}^{n \times n}$.

- There exists an $\mathbf{x} \in \mathbb{R}^n \setminus \{\mathbf{0}\}$ with $\boldsymbol{A}\mathbf{x} = \lambda\mathbf{x}$ (i.e., $(\boldsymbol{A} - \lambda\boldsymbol{I}_n)\mathbf{x} = \mathbf{0}$) that can be solved non-trivially (i.e., $\mathbf{x} \neq \mathbf{0}$).

- $\text{rank}(\boldsymbol{A} - \lambda\boldsymbol{I}_n) < n$.

- $\det(\boldsymbol{A} - \lambda\boldsymbol{I}_n) = 0$.

Remark

- Eigenvectors are NOT unique.

Remark

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- Suppose **x** is an eigenvector of $\boldsymbol{A}$ w.r.t. eigenvalue λ, then for any $c \in \mathbb{R} \setminus \boldsymbol{0}\}$
  $$\boldsymbol{A}(c\mathbf{x}) = c\boldsymbol{A}\mathbf{x} = c\lambda\mathbf{x} = \lambda(c\mathbf{x}).$$

Theorems (or Definitions)

Theorem

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

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Algebraic Multiplicity

Suppose that matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ 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 $\mathrm{am}(\lambda_i)$

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Theorems (or Definitions)

Eigenspace

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

Geometric Multiplicity

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

- Denoted by $\text{gm}(\lambda)$.

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 $\leq$ Algebraic multiplicity

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

$$\text{gm}(\lambda) \leq \text{am}(\lambda).$$

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

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- $\exists \mathbf{v}_{k+1}, \ldots, \mathbf{v}_n$ such that $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ is a basis of $\mathbb{R}^n$.

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- $\exists \mathbf{v}_{k+1}, \ldots, \mathbf{v}_n$ such that $\{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ is a basis of $\mathbb{R}^n$.

- Denote by $\boldsymbol{P} = [\boldsymbol{U} \ \ \boldsymbol{V}]$ for $\boldsymbol{U} = [\mathbf{v}_1 \cdots \mathbf{v}_k]$ and $\boldsymbol{V} = [\mathbf{v}_{k+1} \cdots \mathbf{v}_n]$ (note: $\boldsymbol{P}$ is invertible).

Relation b/w am(λ) & gm(λ) (contd.)

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

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- Then,

$$\begin{bmatrix} \boldsymbol{I}_k & \boldsymbol{O} \\ \boldsymbol{O} & \boldsymbol{I}_{n-k} \end{bmatrix} = \boldsymbol{P}^{-1}\boldsymbol{P} = \begin{bmatrix} \boldsymbol{X} \\ \boldsymbol{Y} \end{bmatrix}[\boldsymbol{U} \ \boldsymbol{V}] = \begin{bmatrix} \boldsymbol{XU} & \boldsymbol{XV} \\ \boldsymbol{YU} & \boldsymbol{YV} \end{bmatrix}$$

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

Relation b/w am(λ) & gm(λ) (contd.)

$$P^{-1}AP = \left[\begin{array}{c} X \\ Y \end{array}\right] A[U \ \ V] = \left[\begin{array}{cc} XAU & XAV \\ YAU & YAV \end{array}\right]$$

Relation b/w am(λ) & gm(λ) (contd.)

$$
\begin{aligned}
\boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{P} &= \left[\begin{array}{c} \boldsymbol{X} \\ \boldsymbol{Y} \end{array}\right] \boldsymbol{A}[\boldsymbol{U}\ \boldsymbol{V}] = \left[\begin{array}{cc} \boldsymbol{XAU} & \boldsymbol{XAV} \\ \boldsymbol{YAU} & \boldsymbol{YAV} \end{array}\right] \\
&= \left[\begin{array}{cc} \lambda\boldsymbol{XU} & \boldsymbol{XAV} \\ \lambda\boldsymbol{YU} & \boldsymbol{YAV} \end{array}\right] = \left[\begin{array}{cc} \lambda\boldsymbol{I}_k & \boldsymbol{XAV} \\ \boldsymbol{O} & \boldsymbol{YAV} \end{array}\right]
\end{aligned}
$$

Relation b/w am(λ) & gm(λ) (contd.)

$$\boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{P} = \left[\begin{array}{c} \boldsymbol{X} \\ \boldsymbol{Y} \end{array}\right] \boldsymbol{A}[\boldsymbol{U} \ \boldsymbol{V}] = \left[\begin{array}{cc} \boldsymbol{X}\boldsymbol{A}\boldsymbol{U} & \boldsymbol{X}\boldsymbol{A}\boldsymbol{V} \\ \boldsymbol{Y}\boldsymbol{A}\boldsymbol{U} & \boldsymbol{Y}\boldsymbol{A}\boldsymbol{V} \end{array}\right]$$

$$= \left[\begin{array}{cc} \lambda\boldsymbol{X}\boldsymbol{U} & \boldsymbol{X}\boldsymbol{A}\boldsymbol{V} \\ \lambda\boldsymbol{Y}\boldsymbol{U} & \boldsymbol{Y}\boldsymbol{A}\boldsymbol{V} \end{array}\right] = \left[\begin{array}{cc} \lambda\boldsymbol{I}_k & \boldsymbol{X}\boldsymbol{A}\boldsymbol{V} \\ \boldsymbol{O} & \boldsymbol{Y}\boldsymbol{A}\boldsymbol{V} \end{array}\right]$$

$$\det(\boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{P} - z\boldsymbol{I}) = \det\left[\begin{array}{cc} \lambda\boldsymbol{I}_k - z\boldsymbol{I}_k & \boldsymbol{X}\boldsymbol{A}\boldsymbol{V} \\ \boldsymbol{O} & \boldsymbol{Y}\boldsymbol{A}\boldsymbol{V} - z\boldsymbol{I}_{n-k} \end{array}\right]$$

Relation b/w am(λ) & gm(λ) (contd.)

$$P^{-1}AP = \left[\begin{array}{c} X \\ Y \end{array} \right] A[U \ V] = \left[\begin{array}{cc} XAU & XAV \\ YAU & YAV \end{array} \right]$$

$$= \left[\begin{array}{cc} \lambda XU & XAV \\ \lambda YU & YAV \end{array} \right] = \left[\begin{array}{cc} \lambda I_k & XAV \\ O & YAV \end{array} \right]$$

$$\det(P^{-1}AP - zI) = \det \left[\begin{array}{cc} \lambda I_k - zI_k & XAV \\ O & YAV - zI_{n-k} \end{array} \right]$$

$$= (\lambda - z)^k \det(YAV - zI_{n-k}).$$

- **Note:** $\det(A - zI) = \det(P^{-1}AP - zI)$.

Remark

$$
\begin{aligned}
\mathbf{P}^{-1}\mathbf{A}\mathbf{P} - z\mathbf{I} &= \mathbf{P}^{-1}\mathbf{A}\mathbf{P} - z\mathbf{P}^{-1}\mathbf{P} \\
&= \mathbf{P}^{-1}\mathbf{A}\mathbf{P} - \mathbf{P}^{-1}(z\mathbf{I})\mathbf{P} \\
&= \mathbf{P}^{-1}(\mathbf{A} - z\mathbf{I})\mathbf{P}.
\end{aligned}
$$

Remark

$$
\begin{aligned}
P^{-1}AP - zI &= P^{-1}AP - zP^{-1}P \\
&= P^{-1}AP - P^{-1}(zI)P \\
&= P^{-1}(A - zI)P.
\end{aligned}
$$

Therefore,

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

The Case of the Identity Matrix

Exercise: The Case of the Identity Matrix

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

- what is $p_I(\lambda)$?
- What are its eigenvalues and the associated eigenvectors?
- What are the eigenspaces?

Useful Properties (1/4)

- $\boldsymbol{A}$ and $\boldsymbol{A}^{\top}$ possess the same eigenvalues

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- A and $A^\top$ possess the same eigenvalues but not necessarily the same eigenvectors.

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\begin{aligned}
\boldsymbol{A}\mathbf{x} = \lambda\mathbf{x} \quad &\Leftrightarrow \quad \boldsymbol{A}\mathbf{x} - \lambda\mathbf{x} = \mathbf{0} \\
&\Leftrightarrow \quad (\boldsymbol{A} - \lambda\boldsymbol{I})\mathbf{x} = \mathbf{0} \\
&\Leftrightarrow \quad \mathbf{x} \in \ker(\boldsymbol{A} - \lambda\boldsymbol{I}).
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- Symmetric, positive definite matrices always have positive, real eigenvalues.
  - $\mathbf{x}^\top \boldsymbol{A}\mathbf{x} = \mathbf{x}^\top \lambda\mathbf{x}$

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

Useful Properties (2/4)

Theorem (4.13)

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

Theorem (4.14)

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

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

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

Useful Properties (3/4)

Theorem

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

Proof.

- Assume that $\boldsymbol{A}\mathbf{v} = \lambda\mathbf{v}$ and $\boldsymbol{A}\mathbf{w} = \mu\mathbf{w}$ for two eigenvectors $\mathbf{v}, \mathbf{w} \in V$ corresponding to eigenvalues λ and μ such that $\lambda \neq \mu$.

- $$\begin{aligned} \lambda\langle\mathbf{v}, \mathbf{w}\rangle &= \langle\lambda\mathbf{v}, \mathbf{w}\rangle = \langle\boldsymbol{A}\mathbf{v}, \mathbf{w}\rangle = (\boldsymbol{A}\mathbf{v})^{\top}\mathbf{w} = \mathbf{v}^{\top}\boldsymbol{A}^{\top}\mathbf{w} = \langle\mathbf{v}, \boldsymbol{A}^{\top}\mathbf{w}\rangle \\ &= \langle\mathbf{v}, \boldsymbol{A}\mathbf{w}\rangle = \langle\mathbf{v}, \mu\mathbf{w}\rangle = \mu\langle\mathbf{v}, \mathbf{w}\rangle. \end{aligned}$$

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

  $\square$

Useful Properties (4/4)

Theorem (4.15; Spectral Theorem)

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

Useful Properties (4/4)

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

Example

Consider

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

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Example

Consider

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

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

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Example

Consider

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

Compute $p_A(\lambda) = -(\lambda - 1)^2(\lambda - 7) \Rightarrow \lambda_1 = 1$ (repeated), $\lambda_2 = 7$.

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

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

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- **Note:** Any linear combination of $\mathbf{x}_1$ and $\mathbf{x}_2$ is also an eigenvector of $\boldsymbol{A}$ w.r.t. λ_1.

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- **Note:** Any linear combination of $\mathbf{x}_1$ and $\mathbf{x}_2$ is also an eigenvector of $\boldsymbol{A}$ w.r.t. λ_1.

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

- Use Gram-Schmidt algorithm to construct an orthogonal basis for $\text{span}(\mathbf{x}_1, \mathbf{x}_2)$!

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

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

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

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$$\mathbf{u}_2 = \mathbf{x}_2 - \frac{\mathbf{u}_1\mathbf{u}_1^\top}{\|\mathbf{u}_1\|^2}\mathbf{x}_2 = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}\begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

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

Why is each eigenvalue real?

- **Note:** Define $\mathbf{x}^* = [a_1 - b_1 i, \ a_2 - b_2 i]^\top$ for $\mathbf{x} = [a_1 + b_1 i, \ a_2 + b_2 i]$. And, define $\boldsymbol{A}^* = \{\overline{\boldsymbol{A}}_{ji}\}_{(i,j) \in N \times M}$ for $\boldsymbol{A} \in \mathbb{C}^{m \times n}$.
- **Note:** $\mathbf{x}^* \mathbf{x} \geq 0$.

Given $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ and $\boldsymbol{A}$ is symmetric:
- Assume that $\boldsymbol{A}\mathbf{x} = \lambda \mathbf{x}$ with $\mathbf{x} \neq \mathbf{0}$.

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- Thus, $(\lambda - \bar{\lambda})\mathbf{x}^* \mathbf{x} = 0$. We have $\lambda = \bar{\lambda}$ since $\mathbf{x}^* \mathbf{x} > 0$. $\Rightarrow \quad \lambda \in \mathbb{R}$.

A Practical Example [Page et al. 1999]

- Google uses the eigenvector corresponding to the maximal eigenvalue of a matrix **A** to determine the rank of a page for search.
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- Websites are represented as a huge directed graph (pages: vertices; links: edges).
- Compute the weight (importance) $x_i \geq 0$ 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.
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Outline

Cholesky Decomposition

Cholesky Decomposition

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

$$
\begin{bmatrix}
a_{11} & \cdots & a_{1n} \\
\vdots & \ddots & \vdots \\
a_{n1} & \cdots & a_{nn}
\end{bmatrix}
=
\begin{bmatrix} \end{bmatrix}
\begin{bmatrix} \end{bmatrix}
$$

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

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

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

Example Steps for Cholesky Factorization

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

- $\ell_{11} = \sqrt{a_{11}}$,

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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).

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- Compute determinants efficiently.
  - $\det(\boldsymbol{A}) = \det(\boldsymbol{L}) \det(\boldsymbol{L}^\top) = \det(\boldsymbol{L})^2$.
  - Note: $\det(\boldsymbol{L})$ can be computed efficiently ($\because$ triangular).

Why Cholesky enables Gaussian sampling

Goal: Generate $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, $\boldsymbol{\Sigma} \in \mathbb{R}^{n \times n}$ is symmetric positive definite (SPD).

1. **Start with i.i.d. standard normals.**
   Draw $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \boldsymbol{I}_n)$ (components independent $N(0, 1)$).

2. **Target distribution.**
   We want $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with given mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$.

3. **Cholesky factorization of $\boldsymbol{\Sigma}$.**
   Since $\boldsymbol{\Sigma}$ is SPD, there exists a lower-triangular L such that $\boldsymbol{\Sigma} = LL^{\top}$.

4. **Build the desired correlations.**

   Set $\mathbf{x} = \boldsymbol{\mu} + L\mathbf{z}$. Then $\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu} + L\,\mathbb{E}[\mathbf{z}] = \boldsymbol{\mu}$,

   $$\mathrm{Cov}(\mathbf{x}) = \mathbb{E}\big[(\mathbf{x} - \boldsymbol{\mu})(\mathbf{x} - \boldsymbol{\mu})^{\top}\big] = \mathbb{E}\big[L\mathbf{z}\mathbf{z}^{\top}L^{\top}\big] = L\boldsymbol{I}_n L^{\top} = LL^{\top} = \boldsymbol{\Sigma}.$$

Outline

1. Eigenvalues & Eigenvectors

2. Cholesky Decomposition

3. Eigendecomposition & Diagonalization

Motivation of Diagonalization

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$$\boldsymbol{D} = \begin{bmatrix} c_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & c_n \end{bmatrix}.$$

- **Question:** What are the determinant, cubic, and inverse of $\boldsymbol{D}$?

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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 $\boldsymbol{A} = \boldsymbol{S}^{-1}\boldsymbol{B}\boldsymbol{S}$.

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

Eigenvectors & Diagonalization

- Let $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ and $\lambda_1, \ldots, \lambda_n$ be a set of scalars.

- Let $\mathbf{p}_1, \ldots, \mathbf{p}_n$ be a set of vectors in $\mathbb{R}^n$.

- Let $\boldsymbol{D} \in \mathbb{R}^{n \times n}$ be a diagonal matrix with diagonal entries $\lambda_1, \ldots, \lambda_n$.

We can show that

$$\boldsymbol{AP} = \boldsymbol{PD}.$$

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 $\boldsymbol{A}$.

Proof Sketch of the Claim

We can see that

$$\boldsymbol{AP} = \boldsymbol{A}[\mathbf{p}_1, \ldots, \mathbf{p}_n] = [\boldsymbol{A}\mathbf{p}_1, \ldots, \boldsymbol{A}\mathbf{p}_n],$$

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Thus,

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

Therefore, the columns of $\boldsymbol{P}$ are eigenvectors of $\boldsymbol{A}$.

Are $\mathbf{p}_1, \ldots, \mathbf{p}_n$ linearly independent?

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

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- $\therefore \alpha_1 = \alpha_2 = \cdots = \alpha_n = 0$.

Eigendecomposition (Diagonalization)

Theorem [Eigendecomposition (Diagonalization)]

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

$$\boldsymbol{A} = \boldsymbol{PDP}^{-1},$$

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

if and only if

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

Put it concisely

Theorem

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

- $\boldsymbol{A}$ is diagonalizable.

- $\boldsymbol{A}$ 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 $\boldsymbol{S} \in \mathbb{R}^{n \times n}$.

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Theorem

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

Example

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

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

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Finally we obtain $\boldsymbol{A} = \boldsymbol{PDP}^{-1}$.

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Maclaurin Series

A Maclaurin Series expansion of $f(x)$ is

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

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

$$
\begin{aligned}
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Remarks

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

Discussions