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

ML Math - Linear Algebra

• Matrix decomposition or matrix factorization.

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- Three matrix decompositions will be introduced.

Outline

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

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

Characteristic Polynomial

Characteristic Polynomial

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

$$\begin{aligned}
\rho_{\mathbf{A}}(\lambda) &:= \det(\mathbf{A} - \lambda \mathbf{I}) \\
&= (-1)^{n} (\lambda - \lambda_{1}) \cdots (\lambda - \lambda_{n}) \\
&= c_{0} + c_{1}\lambda + \cdots + c_{n-1}\lambda^{n-1} + (-1)^{n}\lambda^{n},
\end{aligned}$$

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

Note that

•
$$c_0 = \det(\mathbf{A})$$

Characteristic Polynomial

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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

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

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





ML Math - Linear Algebra Eigenvalues & Eigenvectors

Example

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

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

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

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

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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} .

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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 $am(\lambda_i)$

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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 .

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

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- $\exists \mathbf{v}_{k+1}, \dots, \mathbf{v}_n$ 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).

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

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

- : 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 $\mathbf{A}\mathbf{U} = \mathbf{A}[\mathbf{v}_1 \cdots \mathbf{v}_k] = [\mathbf{A}\mathbf{v}_1 \cdots \mathbf{A}\mathbf{v}_k] = [\lambda \mathbf{v}_1 \cdots \lambda \mathbf{v}_k] = \lambda \mathbf{U}$.

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

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

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$$= (\lambda - z)^k \det(\mathbf{Y}\mathbf{A}\mathbf{V} - z\mathbf{I}_{n-k}).$$

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

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Remark

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

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

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

Therefore,

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

The Case of the Identity Matrix

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?

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.

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

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

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

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- 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

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

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

Theorem

If \boldsymbol{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.

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Example

Consider

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

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

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Consider

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

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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 $\mathbf{x}_3 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$.

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

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

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

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ML Math - Linear Algebra Eigenvalues & Eigenvectors

Take
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ML Math - Linear Algebra Eigenvalues & Eigenvectors

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

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

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

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

- 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 $\mathbf{A}^* = \{\overline{\mathbf{A}}_{ji}\}_{(i,j)\in N\times M}$ for $\mathbf{A}\in\mathbb{C}^{m\times n}$.
- Note: $x^*x \ge 0$.

Given $\mathbf{A} \in \mathbb{R}^{n \times n}$ and \mathbf{A} is symmetric:

• Assume that $\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$ with $\mathbf{x} \neq \mathbf{0}$.

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- Assume that $\mathbf{A}\mathbf{x} = \lambda \mathbf{x}$ with $\mathbf{x} \neq \mathbf{0}$. Note that λ could be a complex number and \mathbf{x} is possibly complex.
- $\mathbf{x}^* \mathbf{A} \mathbf{x} = \mathbf{x}^* \lambda \mathbf{x} = \frac{\lambda \mathbf{x}^* \mathbf{x}}{\lambda \mathbf{x}}$.

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

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) $x_i \ge 0$ for a website a_i and get \mathbf{x} .
 - The number of pages pointing to a_i .
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- Goal: x, Ax, A²x, ..., x*

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- 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).

Outline

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

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

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

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

•
$$\ell_{11} = \sqrt{a_{11}}$$
,



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

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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).

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).

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).

- **9** Start with i.i.d. standard normals. Draw $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I}_n)$ (components independent $\mathcal{N}(0, 1)$).
- 2 Target distribution. We want $\mathbf{x} \sim \mathcal{N}(\mu, \Sigma)$ with given mean μ and covariance Σ .
- **3** Cholesky factorization of Σ . Since Σ is SPD, there exists a lower-triangular L such that $\Sigma = LL^{\top}$.
- Build the desired correlations.

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

$$\mathsf{Cov}(\mathsf{x}) = \mathbb{E}[(\mathsf{x} - \mu)(\mathsf{x} - \mu)^{\top}] = \mathbb{E}[\mathsf{Lzz}^{\top} \mathsf{L}^{\top}] = \mathsf{L} \mathsf{I}_n \mathsf{L}^{\top} = \mathsf{L} \mathsf{L}^{\top} = \Sigma.$$

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1 Eigenvalues & Eigenvectors

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

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

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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 $A = S^{-1}BS$.

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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

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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 \boldsymbol{P} are eigenvectors of \boldsymbol{A} .

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

Eigendecomposition (Diagonalization)

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 $\mathbf{S} \in \mathbb{R}^{n \times n}$

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$\mathsf{Theorem}$

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.

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Compute the eigenvalues and eigenvectors.

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

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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 $\mathbf{A}\mathbf{p}_2 = \frac{3}{2}\mathbf{p}_2$.

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

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

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

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- Construct P:

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

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Maclaurin Series

A Maclaurin Series expansion of f(x) is

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

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46 / 49

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

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NTOU, TW) ML Math - Linear Algebra

46 / 49

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

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Indeed.

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

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

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

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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