## 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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- 2 Cholesky Decomposition
- 3 Eigendecomposition & Diagonalization

## 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  $\boldsymbol{A}$ .

Note that

• 
$$c_0 = \det(\mathbf{A})$$

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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:

- $\lambda$  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  $\lambda$ , 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  $\lambda$  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  $\lambda_i$ . The algebraic multiplicity of  $\lambda_i$  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  $\lambda$  spans the eigenspace of  $\mathbf{A}$  (denoted by  $E_{\lambda}$ ).

### Geometric Multiplicity

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

• 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( $\lambda$ ) & gm( $\lambda$ )

### Geometric multiplicity Algebraic multiplicity

Given  $\mathbf{A} \in \mathbb{R}^{n \times n}$  and assume that  $\lambda$  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  $E_{\lambda}$  such that  $\mathbf{v}_1, \dots, \mathbf{v}_k$  are eigenvectors w.r.t.  $\lambda$ .

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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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- Then,

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

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• 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

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

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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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  - $\mathbf{x}^{\mathsf{T}} \mathbf{A} \mathbf{x} = \mathbf{x}^{\mathsf{T}} \lambda \mathbf{x}$



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

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

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• 
$$E_1 = \operatorname{span}(\mathbf{x}_1, \mathbf{x}_2)$$
, 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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   A w.r.t. λ<sub>1</sub>.

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

 Use Gram-Schmidt algorithm to construct an orthogonal basis for span(x<sub>1</sub>, x<sub>2</sub>)!

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

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,

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

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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 [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.
  - The PageRank algorithm was developed at Stanford University by Larry Page and Sergey Brin in 1996.

### 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.
  - 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, A<sup>2</sup>x, ..., x\*

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- 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).

### 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  $\ell_{11}, \ldots, \ell_{33}$ .

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

• 
$$\ell_{11} = \sqrt{a_{11}}$$
,

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

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

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

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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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- Symmetric positive definite matrices require frequent manipulation.
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- 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).

- 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  $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  with given mean  $\boldsymbol{\mu}$  and covariance  $\boldsymbol{\Sigma}$ .
- **3** Cholesky factorization of  $\Sigma$ . Since  $\Sigma$  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  $\mathbb{E}[\mathbf{x}] = \boldsymbol{\mu} + L\mathbb{E}[\mathbf{z}] = \boldsymbol{\mu}$ ,

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

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1 Eigenvalues & Eigenvectors

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- Diagonalization allow fast computation of determinants, powers and inverses of matrices. A diagonal matrix is like

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

### Similarity

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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  $\boldsymbol{A}$ .

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

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

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

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- $\Rightarrow$  (\*\*)  $-\lambda_n \cdot (*)$ :

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

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

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

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

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

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- $\textbf{ § Check for independency of } \{\textbf{p}_1,\textbf{p}_2\}. \Longrightarrow \checkmark$
- Construct P:

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  - $\star$  Note that  $\{\mathbf{p}_1,\mathbf{p}_2\}$  forms an orthonormal basis

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  - \* Note that  $\{\mathbf{p}_1, \mathbf{p}_2\}$  forms an orthonormal basis  $\mathbf{P}^{-1} = \mathbf{P}^{\top}$ . (Exercise)

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ight].$$

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

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

• 
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.

# Another Application: Using Maclaurin Series

#### Maclaurin Series

A Maclaurin Series expansion of f(x) is

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

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

4 D > 4 B > 4 E > 4 E > 9 Q Q

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

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

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

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

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Indeed.

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

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

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

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

Compute 
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• Eigenvalues: 0, 1.

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

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

### 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**