

Lecture 4: Matrix Decompositions

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Mathematics for Machine Learning

<https://yung-web.github.io/home/courses/mathml.html>

KAIST EE

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Roadmap

- (1) Determinant and Trace
- (2) Eigenvalues and Eigenvectors
- (3) Cholesky Decomposition
- (4) Eigendecomposition and Diagonalization
- (5) Singular Value Decomposition
- (6) Matrix Approximation
- (7) Matrix Phylogeny

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- How to summarize matrices: determinants and eigenvalues
- How matrices can be decomposed: Cholesky decomposition, diagonalization, singular value decomposition
- How these decompositions can be used for matrix approximation

- (1) Determinant and Trace
- (2) Eigenvalues and Eigenvectors
- (3) Cholesky Decomposition
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- For $\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$, $\mathbf{A}^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$.
- \mathbf{A} is invertible iff $a_{11}a_{22} - a_{12}a_{21} \neq 0$
- Let's define $\det(\mathbf{A}) = a_{11}a_{22} - a_{12}a_{21}$.
- Notation: $\det(\mathbf{A})$ or $|\text{whole matrix}|$
- What about 3×3 matrix? By doing some algebra (e.g., Gaussian elimination),

$$\begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23} \\ - a_{31}a_{22}a_{13} - a_{11}a_{32}a_{23} - a_{21}a_{12}a_{33}$$

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Determinant: Motivation (2)

- Try to find some pattern ...

$$\begin{aligned} & a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23} \\ & - a_{31}a_{22}a_{13} - a_{11}a_{32}a_{23} - a_{21}a_{12}a_{33} = \\ & a_{11}(-1)^{1+1} \det(\mathbf{A}_{1,1}) + a_{12}(-1)^{1+2} \det(\mathbf{A}_{1,2}) \\ & + a_{13}(-1)^{1+3} \det(\mathbf{A}_{1,3}) \end{aligned}$$

- $\mathbf{A}_{k,j}$ is the submatrix of \mathbf{A} that we obtain when deleting row k and column j .

$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$ gives the term $a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix}$
 $\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$ gives the term $a_{12} \left(- \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} \right)$
 $\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$ gives the term $a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$

source: www.cliffsnotes.com

- This is called [Laplace expansion](#).
- Now, we can generalize this and provide the formal definition of determinant.

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Determinant

For a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, for all $j = 1, \dots, n$,

1. Expansion along column j : $\det(\mathbf{A}) = \sum_{k=1}^n (-1)^{k+j} a_{kj} \det(\mathbf{A}_{k,j})$
2. Expansion along row j : $\det(\mathbf{A}) = \sum_{k=1}^n (-1)^{k+j} a_{jk} \det(\mathbf{A}_{j,k})$

- All expansion are equal, so no problem with the definition.
- **Theorem.** $\det(\mathbf{A}) \neq 0 \iff \text{rk}(\mathbf{A}) = n \iff \mathbf{A}$ is invertible.

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Determinant: Properties

- (1) $\det(\mathbf{AB}) = \det(\mathbf{A}) \det(\mathbf{B})$
- (2) $\det(\mathbf{A}) = \det(\mathbf{A}^T)$
- (3) For a regular \mathbf{A} , $\det(\mathbf{A}^{-1}) = 1/\det(\mathbf{A})$
- (4) For two similar matrices \mathbf{A}, \mathbf{A}' (i.e., $\mathbf{A}' = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}$ for some \mathbf{S}), $\det(\mathbf{A}) = \det(\mathbf{A}')$
- (5) For a triangular matrix¹ \mathbf{T} , $\det(\mathbf{T}) = \prod_{i=1}^n T_{ii}$
- (6) Adding a multiple of a column/row to another one does not change $\det(\mathbf{A})$
- (7) Multiplication of a column/row with λ scales $\det(\mathbf{A})$: $\det(\lambda\mathbf{A}) = \lambda^n \det(\mathbf{A})$
- (8) Swapping two rows/columns changes the sign of $\det(\mathbf{A})$
 - Using (5)-(8), Gaussian elimination (reaching a triangular matrix) enables to compute the determinant.

¹This includes diagonal matrices.

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- **Definition.** The trace of a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ is defined as

$$\text{tr}(\mathbf{A}) := \sum_{i=1}^n a_{ii}$$

- $\text{tr}(\mathbf{A} + \mathbf{B}) = \text{tr}(\mathbf{A}) + \text{tr}(\mathbf{B})$
- $\text{tr}(\alpha \mathbf{A}) = \alpha \text{tr}(\mathbf{A})$
- $\text{tr}(\mathbf{I}_n) = n$

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Invariant under Cyclic Permutations

- $\text{tr}(\mathbf{AB}) = \text{tr}(\mathbf{BA})$ for $\mathbf{A} \in \mathbb{R}^{n \times k}$ and $\mathbf{B} \in \mathbb{R}^{k \times n}$
- $\text{tr}(\mathbf{AKL}) = \text{tr}(\mathbf{KLA})$, for $\mathbf{A} \in \mathbb{R}^{a \times k}$, $\mathbf{K} \in \mathbb{R}^{k \times l}$, $\mathbf{L} \in \mathbb{R}^{l \times a}$
- $\text{tr}(\mathbf{xy}^T) = \text{tr}(\mathbf{y}^T \mathbf{x}) = \mathbf{y}^T \mathbf{x} \in \mathbb{R}$
- A linear mapping $\Phi : V \mapsto V$, represented by a matrix \mathbf{A} and another matrix \mathbf{B} .
 - \mathbf{A} and \mathbf{B} use different bases, where $\mathbf{B} = \mathbf{S}^{-1} \mathbf{A} \mathbf{S}$

$$\text{tr}(\mathbf{B}) = \text{tr}(\mathbf{S}^{-1} \mathbf{A} \mathbf{S}) = \text{tr}(\mathbf{A} \mathbf{S} \mathbf{S}^{-1}) = \text{tr}(\mathbf{A})$$

- **Message.** While matrix representations of linear mappings are basis dependent, but their traces are not.

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- **Definition.** For $\lambda \in \mathbb{R}$ and a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$, the characteristic polynomial of \mathbf{A} is defined as:

$$\begin{aligned} p_{\mathbf{A}}(\lambda) &:= \det(\mathbf{A} - \lambda \mathbf{I}) \\ &= c_0 + c_1 \lambda + c_2 \lambda^2 + \cdots + c_{n-1} \lambda^{n-1} + (-1)^n \lambda^n, \end{aligned}$$

where $c_0 = \det(\mathbf{A})$ and $c_{n-1} = (-1)^{n-1} \text{tr}(\mathbf{A})$.

- **Example.** For $\mathbf{A} = \begin{pmatrix} 4 & 2 \\ 1 & 3 \end{pmatrix}$,

$$p_{\mathbf{A}}(\lambda) = \begin{vmatrix} 4 - \lambda & 2 \\ 1 & 3 - \lambda \end{vmatrix} = (4 - \lambda)(3 - \lambda) - 2 \cdot 1$$

- (1) Determinant and Trace
- (2) **Eigenvalues and Eigenvectors**
- (3) Cholesky Decomposition
- (4) Eigendecomposition and Diagonalization
- (5) Singular Value Decomposition
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- (7) Matrix Phylogeny

- **Definition.** Consider a square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$. Then, $\lambda \in \mathbb{R}$ is an eigenvalue of \mathbf{A} and $\mathbf{x} \in \mathbb{R}^n \setminus \{0\}$ is the corresponding eigenvector of \mathbf{A} if

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

- Equivalent statements
 - λ is an eigenvalue.
 - $(\mathbf{A} - \lambda\mathbf{I}_n)\mathbf{x} = 0$ can be solved non-trivially, i.e., $\mathbf{x} \neq 0$.
 - $\text{rk}(\mathbf{A} - \lambda\mathbf{I}_n) < n$.
 - $\det(\mathbf{A} - \lambda\mathbf{I}_n) = 0 \iff$ The characteristic polynomial $p_{\mathbf{A}}(\lambda) = 0$.

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Example

- For $\mathbf{A} = \begin{pmatrix} 4 & 2 \\ 1 & 3 \end{pmatrix}$, $p_{\mathbf{A}}(\lambda) = \begin{vmatrix} 4-\lambda & 2 \\ 1 & 3-\lambda \end{vmatrix} = (4-\lambda)(3-\lambda) - 2 \cdot 1 = \lambda^2 - 7\lambda + 10$
- Eigenvalues $\lambda = 2$ or $\lambda = 5$.
- Eigenvector E_5 for $\lambda = 5$

$$\begin{pmatrix} 4-\lambda & 2 \\ 1 & 3-\lambda \end{pmatrix} \mathbf{x} = 0 \implies \begin{pmatrix} -1 & 2 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0 \implies E_5 = \text{span}\left[\begin{pmatrix} 2 \\ 1 \end{pmatrix}\right]$$
- Eigenvector E_2 for $\lambda = 2$. Similarly, we get $E_2 = \text{span}\left[\begin{pmatrix} 1 \\ -1 \end{pmatrix}\right]$
- **Message.** Eigenvectors are not unique.

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- If \mathbf{x} is an eigenvector of \mathbf{A} , so are all vectors that are collinear².
- E_λ : the set of all eigenvectors for eigenvalue λ , spanning a subspace of \mathbb{R}^n . We call this **eigenspace** of \mathbf{A} for λ .
- E_λ is the solution space of $(\mathbf{A} - \lambda \mathbf{I})\mathbf{x} = 0$, thus $E_\lambda = \ker(\mathbf{A} - \lambda \mathbf{I})$
- **Geometric interpretation**
 - The eigenvector corresponding to a nonzero eigenvalue points in a direction **stretched** by the linear mapping.
 - The eigenvalue is the factor of stretching.
- Identity matrix \mathbf{I} : one eigenvalue $\lambda = 1$ and all vectors $\mathbf{x} \neq 0$ are eigenvectors.

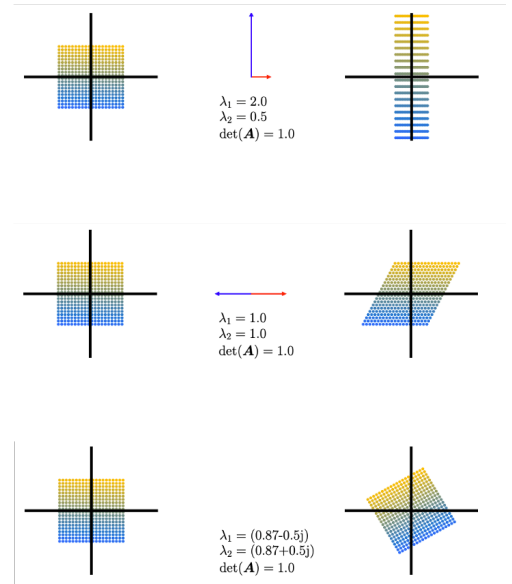
²Two vectors are collinear if they point in the same or the opposite direction.

- \mathbf{A} and \mathbf{A}^T share the eigenvalues, but not necessarily eigenvectors.
- For two similar matrices \mathbf{A}, \mathbf{A}' (i.e., $\mathbf{A}' = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}$ for some \mathbf{S}), they possess the same eigenvalues.
 - Meaning: A linear mapping Φ has eigenvalues that are **independent** of the choice of basis of its transformation matrix.
 - Symmetric, positive definite matrices always have **positive, real** eigenvalues.

determinant, trace, eigenvalues: all **invariant** under basis change

Examples for Geometric Interpretation (1)

1. $\mathbf{A} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{pmatrix}$, $\det(\mathbf{A}) = 1$
 - $\lambda_1 = \frac{1}{2}, \lambda_2 = 2$
 - eigenvectors: canonical basis vectors
 - area preserving, just vertical horizontal) stretching.
2. $\mathbf{A} = \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & 1 \end{pmatrix}$, $\det(\mathbf{A}) = 1$
 - $\lambda_1 = \lambda_2 = 1$
 - eigenvectors: colinear over the horizontal line
 - area preserving, shearing
3. $\mathbf{A} = \begin{pmatrix} \cos(\frac{\pi}{6}) & -\sin(\frac{\pi}{6}) \\ \sin(\frac{\pi}{6}) & \cos(\frac{\pi}{6}) \end{pmatrix}$, $\det(\mathbf{A}) = 1$
 - Rotation by $\pi/6$ counter-clockwise
 - only complex eigenvalues (no eigenvectors)
 - area preserving

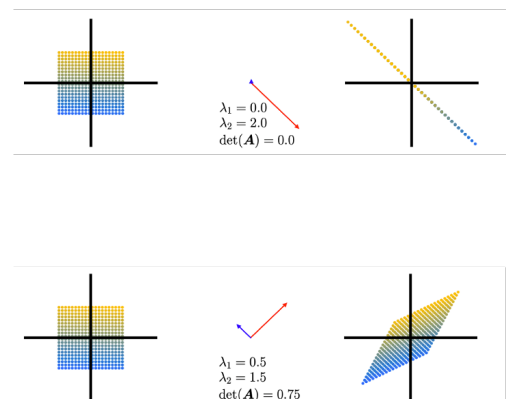


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Examples for Geometric Interpretation (2)

4. $\mathbf{A} = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$, $\det(\mathbf{A}) = 0$
 - $\lambda_1 = 0, \lambda_2 = 2$
 - Mapping that collapses a 2D onto 1D
 - area collapses
5. $\mathbf{A} = \begin{pmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{pmatrix}$, $\det(\mathbf{A}) = 3/4$
 - $\lambda_1 = 0.5, \lambda_2 = 1.5$
 - area scales by 75%, shearing and stretching



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- For $\mathbf{A} \in \mathbb{R}^{n \times n}$, n distinct eigenvalues \implies eigenvectors are linearly independent, which form a basis of \mathbb{R}^n .
 - Converse is not true.
 - Example of n linearly independent eigenvectors for less than n eigenvalues???
- Determinant.** For (possibly repeated) eigenvalues λ_i of $\mathbf{A} \in \mathbb{R}^{n \times n}$,

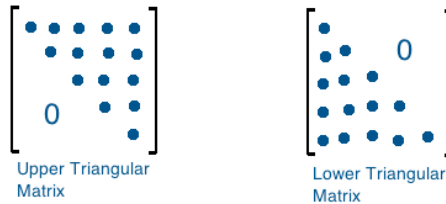
$$\det(\mathbf{A}) = \prod_{i=1}^n \lambda_i$$

- Trace.** For (possibly repeated) eigenvalues λ_i of $\mathbf{A} \in \mathbb{R}^{n \times n}$,

$$\text{tr}(\mathbf{A}) = \sum_{i=1}^n \lambda_i$$

- Message.** $\det(\mathbf{A})$ is the **area scaling** and $\text{tr}(\mathbf{A})$ is the **circumference scaling**

- (1) Determinant and Trace
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Source: <http://mathonline.wikidot.com/>

- The Gaussian elimination is the processing of reaching an upper triangular matrix
- Gaussian elimination: multiplying the matrices corresponding to two elementary operations ((i) row multiplication by a and (ii) adding two rows downward)
- The above elementary operations are the low triangular matrices (LTM), and their inverses and their product are all LTMs.

$$\bullet \quad (\mathbf{E}_k \mathbf{E}_{k-1} \cdots \mathbf{E}_1) \mathbf{A} = \mathbf{U} \implies \mathbf{A} = \underbrace{(\mathbf{E}_1^{-1} \cdots \mathbf{E}_{k-1}^{-1} \mathbf{E}_k^{-1})}_{\mathbf{L}} \mathbf{U}$$

L4(3)

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Cholesky Decomposition

- A real number: decomposition of two identical numbers, e.g., $9 = 3 \times 3$
- **Theorem.** For a symmetric, positive definite matrix \mathbf{A} , $\mathbf{A} = \mathbf{L}\mathbf{L}^T$, where
 - \mathbf{L} is a lower-triangular matrix with positive diagonals
 - Such a \mathbf{L} is unique, called **Cholesky factor** of \mathbf{A} .
- Applications
 - (a) factorization of covariance matrix of a multivariate Gaussian variable
 - (b) linear transformation of random variables
 - (c) fast determinant computation: $\det(\mathbf{A}) = \det(\mathbf{L}) \det(\mathbf{L}^T) = \det(\mathbf{L})^2$, where $\det(\mathbf{L}) = \prod_i l_{ii}$. Thus, $\det(\mathbf{A}) = \prod_i l_{ii}^2$.

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Diagonal Matrix and Diagonalization

- **Diagonal matrix.** zero on all off-diagonal elements, $\mathbf{D} = \begin{pmatrix} d_1 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & d_n \end{pmatrix}$
- $$\mathbf{D}^k = \begin{pmatrix} d_1^k & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & d_n^k \end{pmatrix}, \quad \mathbf{D}^{-1} = \begin{pmatrix} 1/d_1 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 1/d_n \end{pmatrix}, \quad \det(\mathbf{D}) = d_1 d_2 \cdots d_n$$

- **Definition.** $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **diagonalizable** if it is similar to a diagonal matrix \mathbf{D} , i.e., \exists an **invertible** $\mathbf{P} \in \mathbb{R}^{n \times n}$, such that $\mathbf{D} = \mathbf{P}^{-1} \mathbf{A} \mathbf{P}$.
- **Definition.** $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **orthogonally diagonalizable** if it is similar to a diagonal matrix \mathbf{D} , i.e., \exists an **orthogonal** $\mathbf{P} \in \mathbb{R}^{n \times n}$, such that $\mathbf{D} = \mathbf{P}^{-1} \mathbf{A} \mathbf{P} = \mathbf{P}^T \mathbf{A} \mathbf{P}$.

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- $\mathbf{A}^k = \mathbf{P}\mathbf{D}^k\mathbf{P}^{-1}$
- $\det(\mathbf{A}) = \det(\mathbf{P})\det(\mathbf{D})\det(\mathbf{P}^{-1}) = \det(\mathbf{D}) = \prod_i d_{ii}$
- Many other things ...
- **Question.** Under what condition is \mathbf{A} diagonalizable (or orthogonally diagonalizable) and how can we find \mathbf{P} (thus \mathbf{D})?

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Diagonalizability, Algebraic/Geometric Multiplicity

- **Definition.** For a matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ with an eigenvalue λ_i ,
 - the **algebraic multiplicity** α_i of λ_i is the number of times the root appears in the characteristic polynomial.
 - the **geometric multiplicity** ζ_i of λ_i is the number of linearly independent eigenvectors associated with λ_i (i.e., the dimension of the eigenspace spanned by the eigenvectors of λ_i)
- **Example.** The matrix $\mathbf{A} = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}$ has two repeated eigenvalues $\lambda_1 = \lambda_2 = 2$, thus $\alpha_1 = 2$. However, it has only one distinct unit eigenvector $\mathbf{x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, thus $\zeta_1 = 1$.
- **Theorem.** $\mathbf{A} \in \mathbb{R}^{n \times n}$ is **diagonalizable** $\iff \sum_i \alpha_i = \sum_i \zeta_i = n$.

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Theorem. $\mathbf{A} \in \mathbb{R}^{n \times n}$ is orthogonally diagonalizable $\iff \mathbf{A}$ is symmetric.

- **Question.** . How to find \mathbf{P} (thus \mathbf{D})?
- **Spectral Theorem.** If $\mathbf{A} \in \mathbb{R}^{n \times n}$ is symmetric,
 - (a) the eigenvalues are all real
 - (b) the eigenvectors to different eigenvalues are perpendicular.
 - (c) there exists an orthogonal eigenbasis
- For (c), from each set of eigenvectors, say $\{\mathbf{x}_1, \dots, \mathbf{x}_k\}$ associated with a particular eigenvalue, say λ_j , we can construct another set of eigenvectors $\{\mathbf{x}'_1, \dots, \mathbf{x}'_k\}$ that are orthonormal, using the Gram-Schmidt process.
- Then, all eigenvectors can form an orthonormal basis.

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Example

- **Example.** $\mathbf{A} = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{pmatrix}$. $p_{\mathbf{A}}(\lambda) = -(\lambda - 1)^2(\lambda - 7)$, thus $\lambda_1 = 1, \lambda_2 = 7$
 $E_1 = \text{span}\left[\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}\right]$, $E_7 = \text{span}\left[\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\right]$
 - $(111)^T$ is perpendicular to $(-110)^T$ and $(-101)^T$
 - $\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$ and $\begin{pmatrix} -1/2 \\ -1/2 \\ 1 \end{pmatrix}$ (for $\lambda = 1$) and $\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ (for $\lambda = 7$) are the orthogonal basis in \mathbb{R}^3 .
 - After normalization, we can make the orthonormal basis.

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- **Theorem.** The following is equivalent.
 - (a) A square matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$ can be factorized into $\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1}$, where $\mathbf{P} \in \mathbb{R}^{n \times n}$ and \mathbf{D} is the diagonal matrix whose diagonal entries are eigenvalues of \mathbf{A} .
 - (b) The eigenvectors of \mathbf{A} form a basis of \mathbb{R}^n (i.e., The n eigenvectors of \mathbf{A} are linearly independent)
- The above implies the columns of \mathbf{P} are the n eigenvectors of \mathbf{A} (because $\mathbf{A}\mathbf{P} = \mathbf{P}\mathbf{D}$)
- \mathbf{P} is an orthogonal matrix, so $\mathbf{P}^T = \mathbf{P}^{-1}$
- \mathbf{A} is symmetric, then (b) holds (Spectral Theorem).

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Example of Orthogonal Diagonalization (1)

- Eigendecomposition for $\mathbf{A} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$
- Eigenvalues: $\lambda_1 = 1, \lambda_2 = 3$
- (normalized) eigenvectors: $\mathbf{p}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \mathbf{p}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.
- \mathbf{p}_1 and \mathbf{p}_2 linearly independent, so \mathbf{A} is diagonalizable.
- $\mathbf{P} = (\mathbf{p}_1 \ \mathbf{p}_2) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$
- $\mathbf{D} = \mathbf{P}^{-1}\mathbf{A}\mathbf{P} = \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}$. Finally, we get $\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1}$

L4(4)

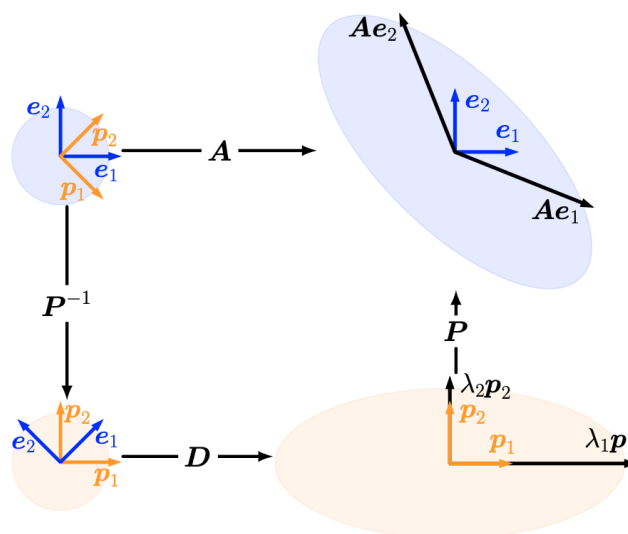
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- $A = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{pmatrix}$
- Eigenvalues: $\lambda_1 = -1, \lambda_2 = 5$
($\alpha_1 = 2, \alpha_2 = 1$)
- $E_{-1} = \text{span}\left[\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}\right] \xrightarrow{\text{Gram-Schmidt}}$
 $\text{span}\left[\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{6}}\begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}\right]$

- $E_5 = \text{span}\left[\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\right]$
- $P = \begin{pmatrix} -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}$
- $D = P^T A P = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 5 \end{pmatrix}$

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Question. Can we generalize this beautiful result to a general matrix $A \in \mathbb{R}^{m \times n}$?

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- (1) Determinant and Trace
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- Eigendecomposition (also called EVD: EigenValue Decomposition): (Orthogonal) Diagonalization for symmetric matrices $\mathbf{A} \in \mathbb{R}^{n \times n}$.
- Extensions: Singular Value Decomposition (SVD)
 1. First extension: diagonalization for non-symmetric, but still square matrices $\mathbf{A} \in \mathbb{R}^{n \times n}$
 2. Second extension: diagonalization for non-symmetric, and non-square matrices $\mathbf{A} \in \mathbb{R}^{m \times n}$
- **Background.** For $\mathbf{A} \in \mathbb{R}^{m \times n}$, a matrix $\mathbf{S} := \mathbf{A}^T \mathbf{A} \in \mathbb{R}^{n \times n}$ is always symmetric, positive semidefinite.
 - Symmetric, because $\mathbf{S}^T = (\mathbf{A}^T \mathbf{A})^T = \mathbf{A}^T \mathbf{A} = \mathbf{S}$.
 - Positive semidefinite, because $\mathbf{x}^T \mathbf{S} \mathbf{x} = \mathbf{x}^T \mathbf{A}^T \mathbf{A} \mathbf{x} = (\mathbf{A} \mathbf{x})^T (\mathbf{A} \mathbf{x}) \geq 0$.
 - If $\text{rk}(\mathbf{A}) = n$, then symmetric and positive definite.

L4(5)

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- **Theorem.** $\mathbf{A} \in \mathbb{R}^{m \times n}$ with rank $r \in [0, \min(m, n)]$. The SVD of \mathbf{A} is a decomposition of the form

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T,$$

$$\begin{matrix} n \\ \boxed{\mathbf{A}} \end{matrix} = \begin{matrix} m \\ \boxed{\mathbf{U}} \end{matrix} \begin{matrix} m \\ \boxed{\mathbf{\Sigma}} \end{matrix} \begin{matrix} n \\ \boxed{\mathbf{V}^T} \end{matrix}$$

with an orthogonal matrix $\mathbf{U} = (\mathbf{u}_1 \cdots \mathbf{u}_m) \in \mathbb{R}^{m \times m}$ and an orthogonal matrix $\mathbf{V} = (\mathbf{v}_1 \cdots \mathbf{v}_n) \in \mathbb{R}^{n \times n}$. Moreover, $\mathbf{\Sigma}$ is an $m \times n$ matrix with $\Sigma_{ii} = \sigma_i \geq 0$ and $\Sigma_{ij} = 0, i \neq j$, which is uniquely determined for \mathbf{A} .

- Note
 - The diagonal entries $\sigma_i, i = 1, \dots, r$ are called **singular values**.
 - \mathbf{u}_i and \mathbf{v}_j are called **left** and **right singular vectors**, respectively.

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SVD: How It Works (for $\mathbf{A} \in \mathbb{R}^{n \times n}$)

- $\mathbf{A} \in \mathbb{R}^{n \times n}$ with rank $r \leq n$. Then, $\mathbf{A}^T \mathbf{A}$ is symmetric.
- Orthogonal diagonalization of $\mathbf{A}^T \mathbf{A}$:

$$\mathbf{A}^T \mathbf{A} = \mathbf{V} \mathbf{D} \mathbf{V}^T.$$

- $\mathbf{D} = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$ and an orthogonal matrix $\mathbf{V} = (\mathbf{v}_1 \cdots \mathbf{v}_n)$, where $\lambda_1 \geq \cdots \geq \lambda_r \geq \lambda_{r+1} = \cdots = \lambda_n = 0$ are the eigenvalues of $\mathbf{A}^T \mathbf{A}$ and $\{\mathbf{v}_i\}$ are orthonormal.
- All λ_i are positive

$$\forall \mathbf{x} \in \mathbb{R}^n, \|\mathbf{A}\mathbf{x}\|^2 = \mathbf{A}\mathbf{x}^T \mathbf{A}\mathbf{x} = \mathbf{x}^T \mathbf{A}^T \mathbf{A}\mathbf{x} = \lambda_i \|\mathbf{x}\|^2$$

- $\text{rk}(\mathbf{A}) = \text{rk}(\mathbf{A}^T \mathbf{A}) = \text{rk}(\mathbf{D}) = r$
- Choose $\mathbf{U}' = (\mathbf{u}_1 \cdots \mathbf{u}_r)$, where

$$\mathbf{u}_i = \frac{\mathbf{A}\mathbf{v}_i}{\sqrt{\lambda_i}}, \quad 1 \leq i \leq r.$$

- We can construct $\{\mathbf{u}_i\}, i = r+1, \dots, n$, so that $\mathbf{U} = (\mathbf{u}_1 \cdots \mathbf{u}_n)$ is an orthonormal basis of \mathbb{R}^n .
- Define $\mathbf{\Sigma} = \begin{pmatrix} \sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n} \end{pmatrix}$
- Then, we can check that $\mathbf{U}\mathbf{\Sigma} = \mathbf{A}\mathbf{V}$.
- Similar arguments for a general $\mathbf{A} \in \mathbb{R}^{m \times n}$ (see pp. 104)

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- $\mathbf{A} = \begin{pmatrix} 1 & 0 & 1 \\ -2 & 1 & 0 \end{pmatrix}$
- $\mathbf{A}^T \mathbf{A} = \begin{pmatrix} 5 & -2 & 1 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \mathbf{V} \mathbf{D} \mathbf{V}^T,$
- $\mathbf{D} = \begin{pmatrix} 6 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \mathbf{V} = \begin{pmatrix} \frac{5}{\sqrt{30}} & \frac{-2}{\sqrt{30}} & \frac{1}{\sqrt{30}} \\ 0 & \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ \frac{-1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix}$
- $\text{rk}(\mathbf{A}) = 2$ because we have two singular values $\sigma_1 = \sqrt{6}$ and $\sigma_2 = 1$
- $\Sigma = \begin{pmatrix} \sqrt{6} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

- $\mathbf{u}_1 = \mathbf{A} \mathbf{v}_1 / \sigma_1 = \begin{pmatrix} \frac{1}{\sqrt{5}} \\ \frac{-2}{\sqrt{5}} \end{pmatrix}$
- $\mathbf{u}_2 = \mathbf{A} \mathbf{v}_2 / \sigma_2 = \begin{pmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{pmatrix}$
- $\mathbf{U} = (\mathbf{u}_1 \ \mathbf{u}_2) = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix}$
- Then, we can see that $\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^T$.

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EVD ($\mathbf{A} = \mathbf{P} \mathbf{D} \mathbf{P}^{-1}$) vs. SVD ($\mathbf{A} = \mathbf{U} \Sigma \mathbf{V}^T$)

- SVD: **always** exists, EVD: **square** matrix and exists if we can find **a basis of eigenvectors** (such as symmetric matrices)
- \mathbf{P} in EVD is **not necessarily orthogonal** (only true for symmetric \mathbf{A}), but \mathbf{U} and \mathbf{V} are **orthogonal** (so representing rotations)
- Both EVD and SVD: (i) basis change in the domain, (ii) independent scaling of each new basis vector and mapping from domain to codomain, (iii) basis change in the codomain. The difference: for SVD, **different vector spaces** of domain and codomain.
- SVD and EVD are closely related through their projections
 - The left-singular (resp. right-singular) vectors of \mathbf{A} are eigenvectors of $\mathbf{A} \mathbf{A}^T$ (resp. $\mathbf{A}^T \mathbf{A}$)
 - The singular values of \mathbf{A} are the square roots of eigenvalues of $\mathbf{A} \mathbf{A}^T$ and $\mathbf{A}^T \mathbf{A}$
 - When \mathbf{A} is symmetric, EVD = SVD (from spectral theorem)

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- When $\text{rk}(\mathbf{A}) = r$, we can construct SVD as the following with only non-zero diagonal entries in Σ :

$$\mathbf{A} = \underbrace{\mathbf{U}}_{m \times r} \underbrace{\Sigma}_{r \times r} \underbrace{\mathbf{V}^T}_{r \times n}$$

- We can even truncate the decomposed matrices, which can be an approximation of \mathbf{A} : for $k < r$

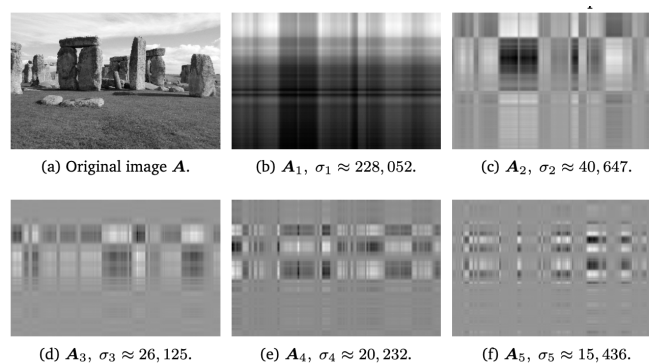
$$\mathbf{A} \approx \underbrace{\mathbf{U}}_{m \times k} \underbrace{\Sigma}_{k \times k} \underbrace{\mathbf{V}^T}_{k \times n}$$

We will cover this in the next slides.

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Matrix Approximation via SVD



- $\mathbf{A} = \sum_{i=1}^r \sigma_i \underbrace{\mathbf{u}_i \mathbf{v}_i^T}_{\mathbf{A}_i}$, where \mathbf{A}_i is the outer product³ of \mathbf{u}_i and \mathbf{v}_i
- Rank k -approximation: $\hat{\mathbf{A}}(k) = \sum_{i=1}^k \sigma_i \mathbf{A}_i$, $k < r$

³If \mathbf{u} and \mathbf{v} are both nonzero, then the outer product matrix $\mathbf{u}\mathbf{v}^T$ always has matrix rank 1. Indeed, the columns of the outer product are all proportional to the first column.

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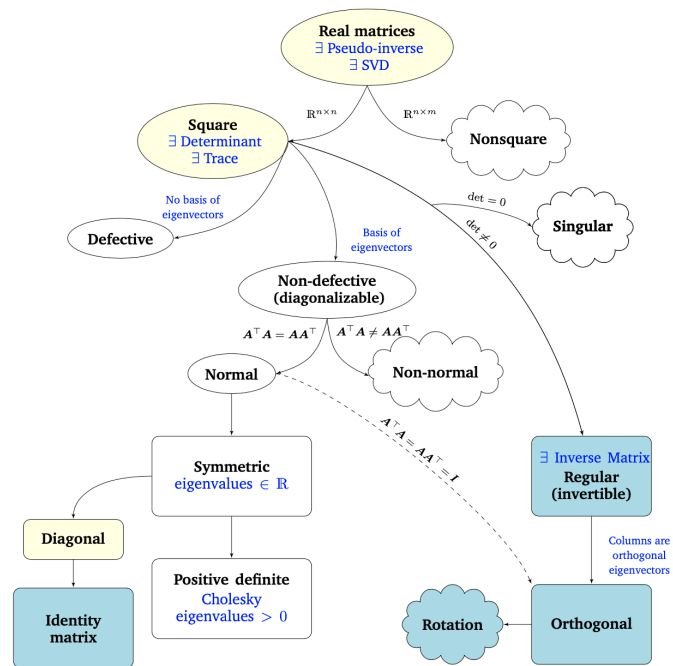
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- **Definition. Spectral Norm of a Matrix.** For $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\|\mathbf{A}\|_2 := \max_{\mathbf{x}} \frac{\|\mathbf{A}\mathbf{x}\|_2}{\|\mathbf{x}\|_2}$
 - As a concept of length of \mathbf{A} , it measures how long any vector \mathbf{x} can at most become, when multiplied by \mathbf{A}
- **Theorem. Eckart-Young.** For $\mathbf{A} \in \mathbb{R}^{m \times n}$ of rank r and $\mathbf{B} \in \mathbb{R}^{m \times n}$ of rank k , for any $k \leq r$, we have:

$$\hat{\mathbf{A}}(k) = \arg \min_{\text{rk}(\mathbf{B})=k} \|\mathbf{A} - \mathbf{B}\|_2, \quad \text{and} \quad \|\mathbf{A} - \hat{\mathbf{A}}(k)\|_2 = \sigma_{k+1}$$

- Quantifies how much error is introduced by the SVD-based approximation
- $\hat{\mathbf{A}}(k)$ is optimal in the sense that such SVD-based approximation is the best one among all rank- k approximations.
- In other words, it is a projection of the full-rank matrix \mathbf{A} onto a lower-dimensional space of rank-at-most- k matrices.

- (1) Determinant and Trace
- (2) Eigenvalues and Eigenvectors
- (3) Cholesky Decomposition
- (4) Eigendecomposition and Diagonalization
- (5) Singular Value Decomposition
- (6) Matrix Approximation
- (7) **Matrix Phylogeny**



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Questions?

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