Lecture 4: Matrix Decompositions

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

- 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

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- For $\boldsymbol{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$, $\boldsymbol{A}^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$.

- $\boldsymbol{A}$ is invertible iff $a_{11}a_{22} - a_{12}a_{21} \neq 0$

- Let's define $\det(\boldsymbol{A}) = a_{11}a_{22} - a_{12}a_{21}$.

- Notation: $\det(\boldsymbol{A})$ or |whole matrix|

- What about 3×3 matrix? By doing some algebra (e.g., Gaussian elimination),

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

$$- a_{31}a_{22}a_{13} - a_{11}a_{32}a_{23} - a_{21}a_{12}a_{33}$$

- Try to find some pattern ...

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

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

source: www.cliffsnotes.com

- This is called Laplace expansion.

- Now, we can generalize this and provide the formal definition of determinant.

Determinant: Formal Definition

Determinant

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

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

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

- All expansion are equal, so no problem with the definition.

- Theorem. $\det(\boldsymbol{A}) \neq 0 \iff \mathrm{rk}(\boldsymbol{A}) = n \iff \boldsymbol{A}$ is invertible.

Determinant: Properties

(1) $\det(\boldsymbol{AB}) = \det(\boldsymbol{A}) \det(\boldsymbol{B})$

(2) $\det(\boldsymbol{A}) = \det(\boldsymbol{A}^{\mathsf{T}})$

(3) For a regular $\boldsymbol{A}$, $\det(\boldsymbol{A}^{-1}) = 1/\det(\boldsymbol{A})$

(4) For two similar matrices $\boldsymbol{A}, \boldsymbol{A}'$ (i.e., $\boldsymbol{A}' = \boldsymbol{S}^{-1}\boldsymbol{AS}$ for some $\boldsymbol{S}$), $\det(\boldsymbol{A}) = \det(\boldsymbol{A}')$

(5) For a triangular matrix[1] $\boldsymbol{T}$, $\det(\boldsymbol{T}) = \prod_{i=1}^{n} T_{ii}$

(6) Adding a multiple of a column/row to another one does not change $\det(\boldsymbol{A})$

(7) Multiplication of a column/row with λ scales $\det(\boldsymbol{A})$: $\det(\lambda\boldsymbol{A}) = \lambda^n \boldsymbol{A}$

(8) Swapping two rows/columns changes the sign of $\det(\boldsymbol{A})$

- Using (5)-(8), Gaussian elimination (reaching a triangular matrix) enables to compute the determinant.

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[1]This includes diagonal matrices.

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

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

- $\text{tr}(A + B) = \text{tr}(A) + \text{tr}(B)$

- $\text{tr}(\alpha A) = \alpha \, \text{tr}(A)$

- $\text{tr}(I_n) = n$

- $\text{tr}(AB) = \text{tr}(BA)$ for $A \in \mathbb{R}^{n \times k}$ and $B \in \mathbb{R}^{k \times n}$

- $\text{tr}(AKL) = \text{tr}(KLA)$, for $A \in \mathbb{R}^{a \times k}$, $K \in \mathbb{R}^{k \times l}$, $L \in \mathbb{R}^{l \times a}$

- $\text{tr}(xy^\top) = \text{tr}(y^\top x) = y^\top x \in \mathbb{R}$

- A linear mapping $\Phi : V \mapsto V$, represented by a matrix A and another matrix B.
  - A and B use different bases, where $B = S^{-1}AS$

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

  - 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 $\boldsymbol{A} \in \mathbb{R}^{n \times n}$, the characteristic polynomial of $\boldsymbol{A}$ is defined as:

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

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

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

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

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(1) Determinant and Trace

(2) **Eigenvalues and Eigenvectors**

(3) Cholesky Decomposition

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Eigenvalue and Eigenvector

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

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

- Equivalent statements
  - λ is an eigenvalue.

  - $(\boldsymbol{A} - \lambda\boldsymbol{I}_n)\boldsymbol{x} = 0$ can be solved non-trivially, i.e., $\boldsymbol{x} \neq 0$.

  - $\mathrm{rk}(\boldsymbol{A} - \lambda\boldsymbol{I}_n) < n$.

  - $\det(\boldsymbol{A} - \lambda\boldsymbol{I}_n) = 0 \iff$ The characteristic polynomial $p_{\boldsymbol{A}}(\lambda) = 0$.

Example

- For $\boldsymbol{A} = \begin{pmatrix} 4 & 2 \\ 1 & 3 \end{pmatrix}$, $p_{\boldsymbol{A}}(\lambda) = \begin{vmatrix} 4 - \lambda & 2 \\ 1 & 3 - \lambda \end{vmatrix} = (4 - \lambda)(3 - \lambda) - 2 \cdot 1 = \lambda^2 - 7\lambda + 10$

- Eigenvalues $\lambda = 2$ or $\lambda = 5$.

- Eigenvector E_5 for $\lambda = 5$

$$\begin{pmatrix} 4 - \lambda & 2 \\ 1 & 3 - \lambda \end{pmatrix} \boldsymbol{x} = 0 \implies \begin{pmatrix} -1 & 2 \\ 1 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = 0 \implies E_5 = \mathrm{span}[\begin{pmatrix} 2 \\ 1 \end{pmatrix}]$$

- Eigenvector E_2 for $\lambda = 2$. Similarly, we get $E_2 = \mathrm{span}[\begin{pmatrix} 1 \\ -1 \end{pmatrix}]$

- Message. Eigenvectors are not unique.

- If x is an eigenvector of A, so are all vectors that are collinear[2].

- E_λ: the set of all eigenvectors for eigenvalue λ, spanning a subspace of $\mathbb{R}^n$. We call this eigensapce of A for λ.

- E_λ is the solution space of $(A - \lambda I)x = 0$, thus $E_\lambda = \ker(A - \lambda I)$

- 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 I: one eigvenvalue $\lambda = 1$ and all vectors $x \neq 0$ are eigenvectors.

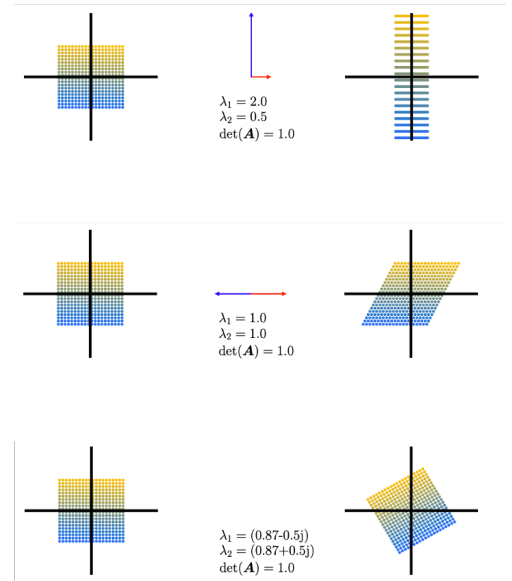[2]Two vectors are collinear if they point in the same or the opposite direction.

- A and A^{T} share the eigenvalues, but not necessarily eigenvectors.

- For two similar matrices A, A' (i.e., $A' = S^{-1}AS$ for some 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. $\boldsymbol{A} = \left(\begin{smallmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{smallmatrix} \right)$, $\det(\boldsymbol{A}) = 1$
   - $\lambda_1 = \frac{1}{2}, \lambda_2 = 2$
     - eigenvectors: canonical basis vectors
     - area preserving, just vertical horizontal) stretching.
2. $\boldsymbol{A} = \left(\begin{smallmatrix} 1 & \frac{1}{2} \\ 0 & 1 \end{smallmatrix} \right)$, $\det(\boldsymbol{A}) = 1$
   - $\lambda_1 = \lambda_2 = 1$
     - eigenvectors: colinear over the horiontal line
     - area preserving, shearing
3. $\boldsymbol{A} = \left(\begin{smallmatrix} \cos(\frac{\pi}{6}) & -\sin(\frac{\pi}{6}) \\ \sin(\frac{\pi}{6}) & \cos(\frac{\pi}{6}) \end{smallmatrix} \right)$, $\det(\boldsymbol{A}) = 1$
   - Rotation by $\pi/6$ counter-clockwise
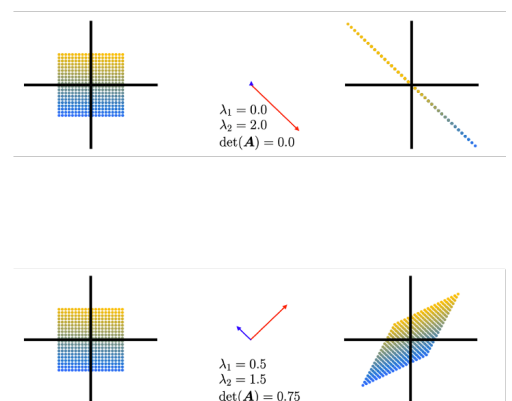   - only complex eigenvalues (no eigenvectors)
     - area preserving

$\lambda_1 = 2.0$
$\lambda_2 = 0.5$
$\det(\boldsymbol{A}) = 1.0$

$\lambda_1 = 1.0$
$\lambda_2 = 1.0$
$\det(\boldsymbol{A}) = 1.0$

$\lambda_1 = (0.87\text{-}0.5j)$
$\lambda_2 = (0.87\text{+}0.5j)$
$\det(\boldsymbol{A}) = 1.0$

Examples for Geometric Interpretation (2)

4. $\boldsymbol{A} = \left(\begin{smallmatrix} 1 & -1 \\ -1 & 1 \end{smallmatrix} \right)$, $\det(\boldsymbol{A}) = 0$
   - $\lambda_1 = 0, \lambda_2 = 2$
     - Mapping that collapses a 2D onto 1D
     - area collapses

5. $\boldsymbol{A} = \left(\begin{smallmatrix} 1 & \frac{1}{2} \\ \frac{1}{2} & 1 \end{smallmatrix} \right)$, $\det(\boldsymbol{A}) = 3/4$
   - $\lambda_1 = 0.5, \lambda_2 = 1.5$
     - area scales by 75%, shearing and stretching

$\lambda_1 = 0.0$
$\lambda_2 = 2.0$
$\det(\boldsymbol{A}) = 0.0$

$\lambda_1 = 0.5$
$\lambda_2 = 1.5$
$\det(\boldsymbol{A}) = 0.75$

Properties (3)

- For $\boldsymbol{A} \in \mathbb{R}^{n \times n}$, 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 $\boldsymbol{A} \in \mathbb{R}^{n \times n}$,

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

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

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

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

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Upper Triangular Matrix   Lower Triangular Matrix

Source: http://mathonline.wikidot.com/
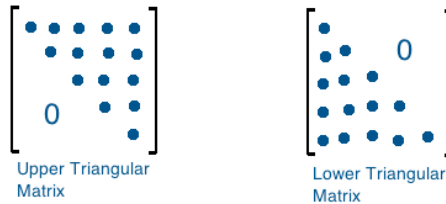
- The Gaussian elimination is the processing of reaching an upper triangular matrix

- 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.

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

- A real number: decomposition of two identical numbers, e.g., $9 = 3 \times 3$

- Theorem. For a symmetric, positive definite matrix $\boldsymbol{A}$, $\boldsymbol{A} = \boldsymbol{L}\boldsymbol{L}^{\mathsf{T}}$, where
  - $\boldsymbol{L}$ is a lower-triangular matrix with positive diagonals
  - Such a $\boldsymbol{L}$ is unique, called Cholesky factor of $\boldsymbol{A}$.

- Applications
  (a) factorization of covariance matrix of a multivariate Gaussian variable
  (b) linear transformation of random variables
  (c) fast determinant computation: $\det(\boldsymbol{A}) = \det(\boldsymbol{L})\det(\boldsymbol{L}^{\mathsf{T}}) = \det(\boldsymbol{L})^2$, where $\det(\boldsymbol{L}) = \prod_i l_{ii}$. Thus, $\det(\boldsymbol{A}) = \prod_i l_{ii}^2$.

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Diagonal Matrix and Diagonalization

- Diagonal matrix. zero on all off-diagonal elements, $\boldsymbol{D} = \begin{pmatrix} d_1 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & d_n \end{pmatrix}$

$$\boldsymbol{D}^k = \begin{pmatrix} d_1^k & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & d_n^k \end{pmatrix}, \quad \boldsymbol{D}^{-1} = \begin{pmatrix} 1/d_1 & \cdots & 0 \\ \vdots & & \vdots \\ 0 & \cdots & 1/d_n \end{pmatrix}, \quad \det(\boldsymbol{D}) = d_1 d_2 \cdots d_n$$

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

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

Power of Diagonalization

- $\boldsymbol{A}^k = \boldsymbol{P}\boldsymbol{D}^k\boldsymbol{P}^{-1}$

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

- Many other things ...

- Question. Under what condition is $\boldsymbol{A}$ diagonalizable (or orthogonally diagonalizable) and how can we find $\boldsymbol{P}$ (thus $\boldsymbol{D}$)?

Diagonalizablity, Algebraic/Geometric Multiplicity

- Definition. For a matrix $\boldsymbol{A} \in$ *realnn* 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 $\boldsymbol{A} = \begin{pmatrix} 2 & 1 \\ 0 & 2 \end{pmatrix}$ has two repeated eigenvalues $\lambda_1 = \lambda_2 = 2$, thus $\alpha_1 = 2$. However, it has only one distinct unit eigenvector $\boldsymbol{x} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, thus $\zeta_1 = 1$.

- Theorem. $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is diagonalizable $\iff \sum_i \alpha_i = \sum_i \zeta_i = n$.

Orthogonally Diagonaliable and Symmetric Matrix

> **Theorem.** $A \in \mathbb{R}^{n \times n}$ is orthogonally diagonalizable $\Longleftrightarrow$ A is symmetric.

- **Question.** . How to find P (thus D)?

- **Spectral Theorem.** If $A \in \mathbb{R}^{n \times n}$ 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 $\{x_1, \ldots, x_k\}$ associated with a particular eigenvalue, say λ_j, we can construct another set of eigenvectors $\{x'_1, \ldots, x'_k\}$ that are orthonormal, using the Gram-Schmidt process.

- Then, all eigenvectors can form an orthornormal basis.

Example

- **Example.** $A = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & 2 \\ 2 & 2 & 3 \end{pmatrix}$. $p_A(\lambda) = -(\lambda - 1)^2(\lambda - 7)$, thus $\lambda_1 = 1, \lambda_2 = 7$

  $E_1 = \text{span}[\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}], \quad E_7 = \text{span}[\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}]$

  ◦ $(111)^{\mathsf{T}}$ is perpendicular to $(-110)^{\mathsf{T}}$ and $(-101)^{\mathsf{T}}$

  ◦ $\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$ 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.

Eigendecomposition

- **Theorem.** The following is equivalent.
  - (a) A square matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ can be factorized into $\boldsymbol{A} = \boldsymbol{P}\boldsymbol{D}\boldsymbol{P}^{-1}$, where $\boldsymbol{P} \in \mathbb{R}^{n \times n}$ and $\boldsymbol{D}$ is the diagonal matrix whose diagonal entries are eigenvalues of $\boldsymbol{A}$.

  - (b) The eigenvectors of $\boldsymbol{A}$ form a basis of $\mathbb{R}^n$ (i.e., The n eigenvectors of $\boldsymbol{A}$ are linearly independent)

- The above implies the columns of $\boldsymbol{P}$ are the n eigenvectors of $\boldsymbol{A}$ (because $\boldsymbol{A}\boldsymbol{P} = \boldsymbol{P}\boldsymbol{D}$)

- $\boldsymbol{P}$ is an orthogonal matrix, so $\boldsymbol{P}^{\mathsf{T}} = \boldsymbol{P}^{-1}$

- $\boldsymbol{A}$ is symmetric, then (b) holds (Spectral Theorem).

Example of Orthogonal Diagonalization (1)

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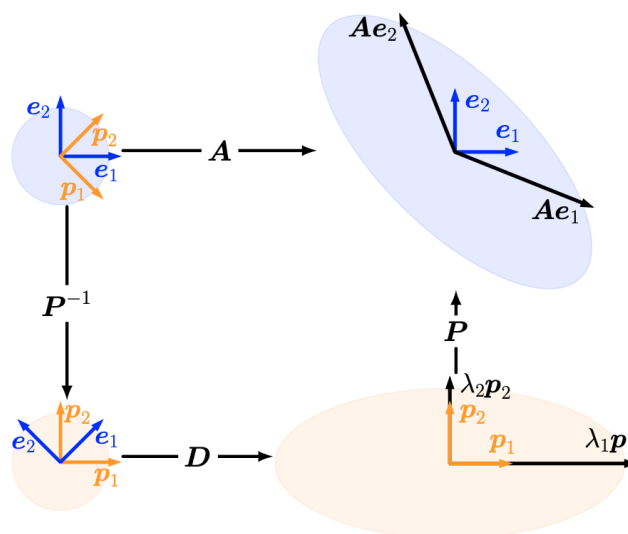
- $A = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{pmatrix}$

- Eigenvalues: $\lambda_1 = -1, \lambda_2 = 5$
  $(\alpha_1 = 2, \alpha_2 = 1)$

- $E_{-1} = \text{span}[\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}] \xrightarrow{\text{Gram-Schmidt}}$

  $\text{span}[\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{6}}\begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}]$

- $E_5 = \text{span}[\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}]$

- $P = \begin{pmatrix} -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}$

- $D = P^\mathsf{T} A P = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 5 \end{pmatrix}$

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

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- Eigendecomposition (also called EVD: EigenValue Decomposition): (Orthogoanl) Diagonalization for symmetric matrices $\boldsymbol{A} \in \mathbb{R}^{n \times n}$.

- Extensions: Singular Value Decomposition (SVD)
    1. First extension: diagonalization for non-symmetric, but still square matrices $\boldsymbol{A} \in \mathbb{R}^{n \times n}$
    2. Second extension: diagonalization for non-symmeric, and non-square matrices $\boldsymbol{A} \in \mathbb{R}^{m \times n}$

- Background. For $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, a matrix $\boldsymbol{S} := \boldsymbol{A}^\mathsf{T} \boldsymbol{A} \in \mathbb{R}^{n \times n}$ is always symmetric, positive semidefinite.
    - Symmetric, because $\boldsymbol{S}^\mathsf{T} = \left(\boldsymbol{A}^\mathsf{T} \boldsymbol{A}\right)^\mathsf{T} = \boldsymbol{A}^\mathsf{T} \boldsymbol{A} = \boldsymbol{S}$.
    - Positive semidefinite, because $\boldsymbol{x}^\mathsf{T} \boldsymbol{S} \boldsymbol{x} = \boldsymbol{x}^\mathsf{T} \boldsymbol{A}^\mathsf{T} \boldsymbol{A} \boldsymbol{x} = \left(\boldsymbol{A}\boldsymbol{x}\right)^\mathsf{T}\left(\boldsymbol{A}\boldsymbol{x}\right) \geq 0$.
    - If $\mathrm{rk}(\boldsymbol{A}) = n$, then symmetric and positive definite.

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

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

with an orthogonal matrix $U = \begin{pmatrix} u_1 & \cdots & u_m \end{pmatrix} \in \mathbb{R}^{m \times m}$ and an orthogonal matrix $V = \begin{pmatrix} v_1 & \cdots & v_n \end{pmatrix} \in \mathbb{R}^{n \times n}$. Moreoever, Σ s an $m \times n$ matrix with $\Sigma_{ii} = \sigma_i \geq 0$ and $\Sigma_{ij} = 0$, $i \neq j$, which is uniquely determined for A.

- Note
  - The diagonal entries σ_i, $i = 1, \ldots, r$ are called singular values.
  - u_i and v_j are called left and right singular vectors, respectively.

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

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

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

- $D = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$ and an orthogonal matrix $V = \begin{pmatrix} v_1 \cdots v_n \end{pmatrix}$, where $\lambda_1 \geq \cdots \geq \lambda_r \geq \lambda_{r+1} = \cdots \lambda_n = 0$ are the eigenvalues of $A^\mathsf{T} A$ and $\{v_i\}$ are orthonormal.

- All λ_i are positive
  $\forall x \in \mathbb{R}^n, \|Ax\|^2 = Ax^\mathsf{T} Ax = x^\mathsf{T} A^\mathsf{T} Ax = \lambda_i \|x\|^2$

- rk(A) =rk($A^\mathsf{T} A$) = rk(D) =r
- Choose $U' = \begin{pmatrix} u_1 & \cdots u_r \end{pmatrix}$, where

$$u_i = \frac{Av_i}{\sqrt{\lambda_i}}, \ 1 \leq i \leq r.$$

- We can construct $\{u_i\}$, $i = r+1, \cdots, n$, so that $U = \begin{pmatrix} u_1 & \cdots u_n \end{pmatrix}$ is an orthonormal basis of $\mathbb{R}^n$.

- Define $\Sigma = \begin{pmatrix} \sqrt{\lambda_1} & & \\ & \ddots & \\ & & \sqrt{\lambda_n} \end{pmatrix}$

- Then, we can check that $U\Sigma = AV$.
- Similar arguments for a general $A\mathbb{R}^{m \times n}$ (see pp. 104)

- $A = \begin{pmatrix} 1 & 0 & 1 \\ -2 & 1 & 0 \end{pmatrix}$

- $A^{\mathsf{T}}A = \begin{pmatrix} 5 & -2 & 1 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} = VDV^{\mathsf{T}},$

- $D = \begin{pmatrix} 6 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, V = \begin{pmatrix} \frac{5}{\sqrt{30}} & \frac{-2}{\sqrt{30}} & \frac{1}{\sqrt{30}} \\ 0 & \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ \frac{-1}{\sqrt{6}} & \frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{6}} \end{pmatrix}$

- $\mathrm{rk}(A) = 2$ because we have two singular values $\sigma_1 = \sqrt{6}$ and $\sigma_2 = 1$

- $\Sigma = \begin{pmatrix} \sqrt{6} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

- $u_1 = Av_1/\sigma_1 = \begin{pmatrix} \frac{1}{\sqrt{5}} \\ \frac{-2}{\sqrt{5}} \end{pmatrix}$

- $u_2 = Av_2/\sigma_2 = \begin{pmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{pmatrix}$

- $U = \begin{pmatrix} u_1 & u_2 \end{pmatrix} = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix}$

- Then, we can see that $A = U\Sigma V^{\mathsf{T}}$.

EVD ($A = PDP^{-1}$) vs. SVD ($A = U\Sigma V^{\mathsf{T}}$)   KAIST EE

- SVD: always exists, EVD: square matrix and exists if we can find a basis of eigenvectors (such as symmetric matrices)

- P in EVD is not necessarily orthogonal (only true for symmetric A), but U and 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 A are eigenvectors of AA^{T} (resp. $A^{\mathsf{T}}A$)
  - The singular values of A are the square roots of eigenvalues of AA^{T} and $A^{\mathsf{T}}A$
  - When A is symmetric, EVD = SVD (from spectral theorem)

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

$$\boldsymbol{A} = \overbrace{\boldsymbol{U}}^{m \times r} \overbrace{\Sigma}^{r \times r} \overbrace{\boldsymbol{V}^{\mathsf{T}}}^{r \times n}$$

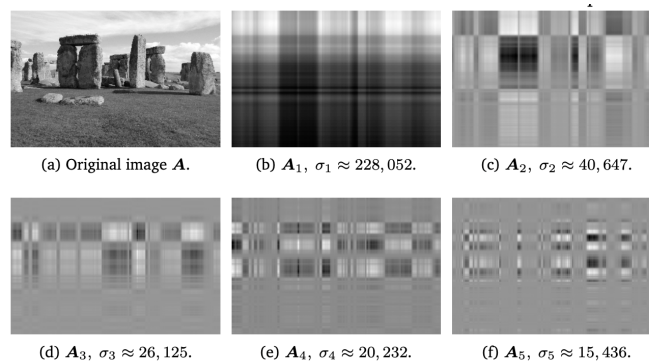- We can even truncate the decomposed matrices, which can be an approximation of $\boldsymbol{A}$: for $k < r$

$$\boldsymbol{A} \approx \overbrace{\boldsymbol{U}}^{m \times k} \overbrace{\Sigma}^{k \times k} \overbrace{\boldsymbol{V}^{\mathsf{T}}}^{k \times n}$$

We will cover this in the next slides

(a) Original image $\boldsymbol{A}$.　　(b) $\boldsymbol{A}_1$, $\sigma_1 \approx 228,052$.　　(c) $\boldsymbol{A}_2$, $\sigma_2 \approx 40,647$.

(d) $\boldsymbol{A}_3$, $\sigma_3 \approx 26,125$.　　(e) $\boldsymbol{A}_4$, $\sigma_4 \approx 20,232$.　　(f) $\boldsymbol{A}_5$, $\sigma_5 \approx 15,436$.

- $\boldsymbol{A} = \sum_{i=1}^{r} \sigma_i \overbrace{\boldsymbol{u}_i \boldsymbol{v}_i^{\mathsf{T}}}^{\boldsymbol{A}_i}$, where $\boldsymbol{A}_i$ is the outer product[3] of $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$

- Rank k-approximation: $\hat{\boldsymbol{A}}(k) = \sum_{i=1}^{k} \sigma_i \boldsymbol{A}_i$, $k < r$

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

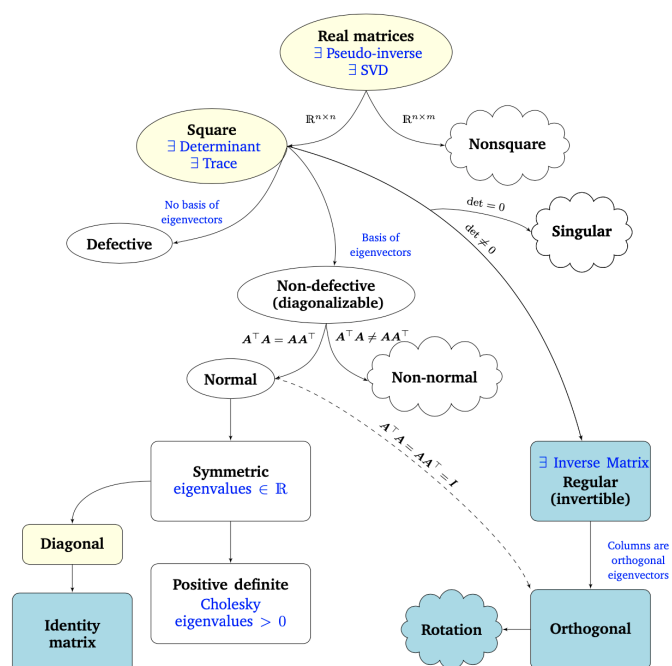- Definition. Spectral Norm of a Matrix. For $A \in \mathbb{R}^{m \times n}$, $\|A\|_2 := \max_x \dfrac{\|Ax\|_2}{\|x\|_2}$

  ◦ As a concept of length of A, it measures how long any vector x can at most become, when multiplied by A

- Theorem. Eckart-Young. For $A \in \mathbb{R}^{m \times n}$ of rank r and $B \in \mathbb{R}^{m \times n}$ of rank k, for any $k \leq r$, we have:

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

  ◦ Quantifies how much error is introduced by the SVD-based approximation

  ◦ $\hat{A}(k)$ 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 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

Questions?

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