Matrix Decompositions - EVD and SVD

Introduction to Optimization for Machine Learning
M1 MLSD/AMSD

October 17, 2023

Roadmap

(1) Determinant and Trace

(2) Eigenvalues and Eigenvectors

(3) Eigendecomposition and Diagonalization

(4) Singular Value Decomposition

(5) Matrix Approximation

Summary

- 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

Determinant: Motivation (1)

- 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),

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

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

Determinant: Motivation (2)

- Try to find some pattern ...

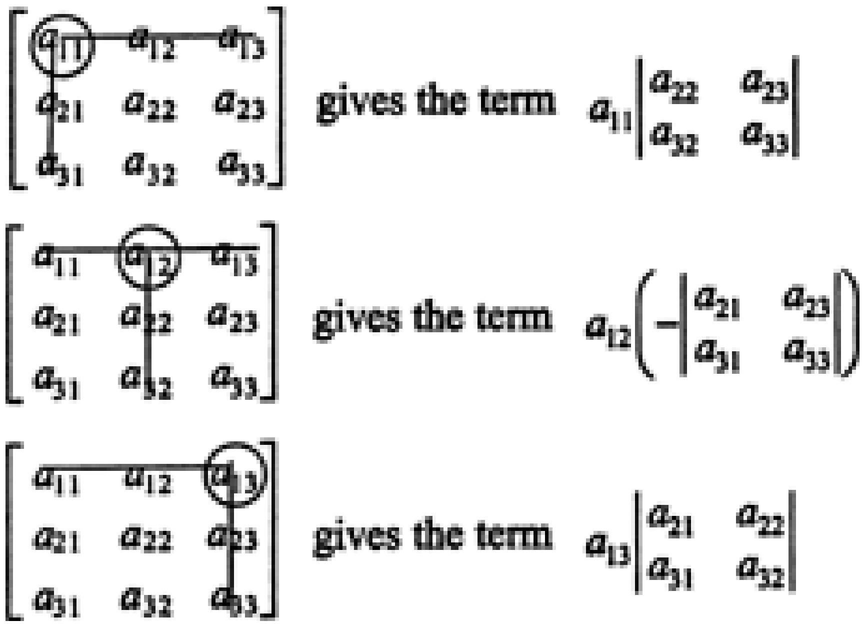
$a_{11}a_{22}a_{33} + a_{21}a_{32}a_{13} + a_{31}a_{12}a_{23}$

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

$a_{11}(-1)^{1+1}\det(\boldsymbol{A}_{1,1}) + a_{12}(-1)^{1+2}\det(\boldsymbol{A}_{1,2})$

$+ a_{13}(-1)^{1+3}\det(\boldsymbol{A}_{1,3})$

- $\boldsymbol{A}_{k,j}$ 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.

[1] This includes diagonal matrices.

Trace

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

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

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

Invariant under Cyclic Permutations

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

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

Background: Characteristic Polynomial

- 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 $c_{n-1} = (-1)^{n-1}\,\mathrm{tr}(\boldsymbol{A})$.

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

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

Roadmap

(1) Determinant and Trace

(2) Eigenvalues and Eigenvectors

(3) Eigendecomposition and Diagonalization

(4) Singular Value Decomposition

(5) Matrix Approximation

Eigenvalue and Eigenvector

- Definition. Consider a square matrix $\boldsymbol{A} \in \mathbb{R}^{n \times n}$. Then, $\lambda \in \mathbb{R}$ 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., $\boldsymbol{x} \neq \boldsymbol{0}$.
  - $\mathrm{rk}(\boldsymbol{A} - \lambda \boldsymbol{I}_n) < n$.
  - $\det(\boldsymbol{A} - \lambda \boldsymbol{I}_n) = 0 \iff$ The characteristic polynomial $p_{\boldsymbol{A}}(\lambda) = 0$.

Example

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

Properties (1)

- If $\boldsymbol{x}$ is an eigenvector of $\boldsymbol{A}$, 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 $\boldsymbol{A}$ for λ.
- 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 $\boldsymbol{I}$: one eigvenvalue $\lambda = 1$ and all vectors $\boldsymbol{x} \neq \boldsymbol{0}$ are eigenvectors.

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

Properties (2)

- $\boldsymbol{A}$ and $\boldsymbol{A}^{\mathsf{T}}$ share the eigenvalues, but not necessarily eigenvectors.
- For two similar matrices $\boldsymbol{A}, \boldsymbol{A}'$ (i.e., $\boldsymbol{A}' = \boldsymbol{S}^{-1}\boldsymbol{A}\boldsymbol{S}$ for some $\boldsymbol{S}$), 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

Properties

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

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

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

Roadmap

(1) Determinant and Trace

(2) Eigenvalues and Eigenvectors

(3) Eigendecomposition and Diagonalization

(4) Singular Value Decomposition

(5) Matrix Approximation

(6) Matrix Phylogeny

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

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 Diagonalizable and Symmetric Matrix

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

- Question. . How to find $\boldsymbol{P}$ (thus $\boldsymbol{D}$)?
- Spectral Theorem. If $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ 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 $\{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_k\}$ associated with a particular eigenvalue, say λ_j, we can construct another set of eigenvectors $\{\boldsymbol{x}'_1, \ldots, \boldsymbol{x}'_k\}$ that are orthonormal, using the Gram-Schmidt process.
- Then, all eigenvectors can form an orthornormal 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 $\boldsymbol{A} = \boldsymbol{P}\boldsymbol{D}\boldsymbol{P}^{-1}$

Example of Orthogonal Diagonalization (2)

- $\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{pmatrix}$
- Eigenvalues: $\lambda_1 = -1, \lambda_2 = 5$ $(\alpha_1 = 2, \alpha_2 = 1)$
- $E_{-1} = \text{span}[\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}] \xrightarrow{\text{Gram-Schmidt}}$ $\text{span}[\frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}, \frac{1}{\sqrt{6}} \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix}]$
- $E_5 = \text{span}[\frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}]$
- $\boldsymbol{P} = \begin{pmatrix} -1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{3} \\ 0 & 2/\sqrt{6} & 1/\sqrt{3} \end{pmatrix}$
- $\boldsymbol{D} = \boldsymbol{P}^\mathsf{T} \boldsymbol{A} \boldsymbol{P} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 5 \end{pmatrix}$

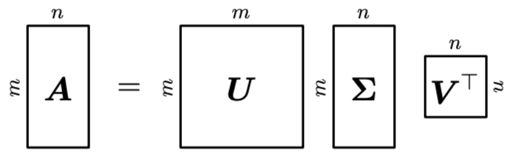
Storyline

- 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 $\boldsymbol{S}^\mathsf{T} = (\boldsymbol{A}^\mathsf{T}\boldsymbol{A})^\mathsf{T} = \boldsymbol{A}^\mathsf{T}\boldsymbol{A} = \boldsymbol{S}$.
  - Positive semidefinite, because $\boldsymbol{x}^\mathsf{T}\boldsymbol{S}\boldsymbol{x} = \boldsymbol{x}^\mathsf{T}\boldsymbol{A}^\mathsf{T}\boldsymbol{A}\boldsymbol{x} = (\boldsymbol{A}\boldsymbol{x})^\mathsf{T}(\boldsymbol{A}\boldsymbol{x}) \geq 0$.
  - If $\mathrm{rk}(\boldsymbol{A}) = n$, then symmetric and positive definite.

Singular Value Decomposition

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

$$\boldsymbol{A} = \boldsymbol{U}\Sigma\boldsymbol{V}^\top,$$



  with an orthogonal matrix $\boldsymbol{U} = \begin{pmatrix}\boldsymbol{u}_1 & \cdots & \boldsymbol{u}_m\end{pmatrix} \in \mathbb{R}^{m\times m}$ and an orthogonal matrix $\boldsymbol{V} = \begin{pmatrix}\boldsymbol{v}_1 & \cdots & \boldsymbol{v}_n\end{pmatrix} \in \mathbb{R}^{n\times n}$. 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 $\boldsymbol{A}$.

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

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

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

$$\boldsymbol{A}^\top \boldsymbol{A} = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^\top.$$

- $\boldsymbol{D} = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$ and an orthogonal matrix $\boldsymbol{V} = \begin{pmatrix} \boldsymbol{v}_1 \cdots \boldsymbol{v}_n \end{pmatrix}$, where $\lambda_1 \ge \cdots \ge \lambda_r \ge \lambda_{r+1} = \cdots \lambda_n = 0$ are the eigenvalues of $\boldsymbol{A}^\top \boldsymbol{A}$ and $\{\boldsymbol{v}_i\}$ are orthonormal.
- All λ_i are positive
- $\mathrm{rk}(\boldsymbol{A})$ $=\mathrm{rk}(\boldsymbol{A}^\top \boldsymbol{A})$ $= \mathrm{rk}(D)$ $=$r
- Choose $\boldsymbol{U}' = \begin{pmatrix} \boldsymbol{u}_1 & \cdots \boldsymbol{u}_r \end{pmatrix}$, where

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

- We can construct $\{\boldsymbol{u}_i\}$, $i = r+1, \cdots, n$, so that $\boldsymbol{U} = \begin{pmatrix} \boldsymbol{u}_1 & \cdots \boldsymbol{u}_n \end{pmatrix}$ 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 $\boldsymbol{U}\Sigma = \boldsymbol{A}\boldsymbol{V}$.
- Similar arguments for a general $\boldsymbol{A}\mathbb{R}^{m\times n}$ (see pp. 104)

Example

- $\boldsymbol{A} = \begin{pmatrix} 1 & 0 & 1 \\ -2 & 1 & 0 \end{pmatrix}$
- $\boldsymbol{A}^\top \boldsymbol{A} = \begin{pmatrix} 5 & -2 & 1 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}^\top,$

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

- $\mathrm{rk}(\boldsymbol{A}) = 2$ because we have two singular values $\sigma_1 = \sqrt{6}$ and $\sigma_2 = 1$
- $\Sigma = \begin{pmatrix} \sqrt{6} & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
- $\boldsymbol{u}_1 = \boldsymbol{A}\boldsymbol{v}_1/\sigma_1 = \begin{pmatrix} \frac{1}{\sqrt{5}} \\ \frac{-2}{\sqrt{5}} \end{pmatrix}$
- $\boldsymbol{u}_2 = \boldsymbol{A}\boldsymbol{v}_2/\sigma_2 = \begin{pmatrix} \frac{2}{\sqrt{5}} \\ \frac{1}{\sqrt{5}} \end{pmatrix}$
- $\boldsymbol{U} = \begin{pmatrix} \boldsymbol{u}_1 & \boldsymbol{u}_2 \end{pmatrix} = \frac{1}{\sqrt{5}} \begin{pmatrix} 1 & 2 \\ -2 & 1 \end{pmatrix}$
- Then, we can see that $\boldsymbol{A} = \boldsymbol{U}\Sigma V^\top$.

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

- SVD: always exists, EVD: square matrix and exists if we can find a basis of eigenvectors (such as symmetric matrices)
- $\boldsymbol{P}$ in EVD is not necessarily orthogonal (only true for symmetric $\boldsymbol{A}$), but $\boldsymbol{U}$ and $\boldsymbol{V}$ 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 $\boldsymbol{A}$ are eigenvectors of $\boldsymbol{A}\boldsymbol{A}^{\mathsf{T}}$ (resp. $\boldsymbol{A}^{\mathsf{T}}\boldsymbol{A}$)
  - The singular values of $\boldsymbol{A}$ are the square roots of eigenvalues of $\boldsymbol{A}\boldsymbol{A}^{\mathsf{T}}$ and $\boldsymbol{A}^{\mathsf{T}}\boldsymbol{A}$
  - When $\boldsymbol{A}$ is symmetric, EVD $=$ SVD (from spectral theorem)

Different Forms of SVD

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

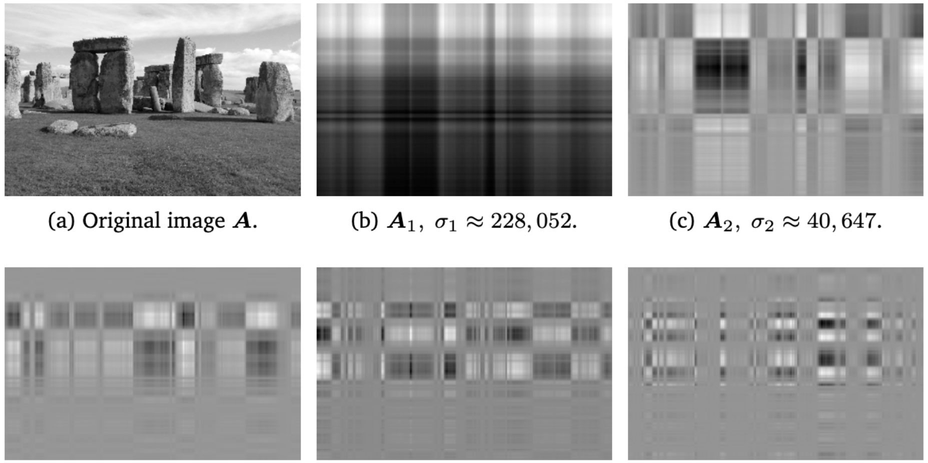
$$\boldsymbol{A} = \overbrace{\boldsymbol{U}}^{m \times r} \overbrace{\boldsymbol{\Sigma}}^{r \times r} \overbrace{\boldsymbol{V}^\mathsf{T}}^{r \times n}$$

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

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

We will cover this in the next slides.

Matrix Approximation via SVD



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

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

How Close $\hat{\boldsymbol{A}}(k)$ is to $\boldsymbol{A}$?

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

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

  - Quantifies how much error is introduced by the SVD-based approximation
  - $\hat{\boldsymbol{A}}(k)$ 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 $\boldsymbol{A}$ onto a lower-dimensional space of rank-at-most-k matrices.