Matrix Decompositions

CoE197M/EE298M (Foundations of Machine Learning)

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Reference: "Mathematics for Machine Learning". Copyright 2020 by Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong. Published by Cambridge University Press.

Matrix Decompositions

- Decomposing a matrix into a product of simpler matrices lets us better understand the data that the matrix represents
 - For example, by decomposing MNIST images, we understand what makes digits 0 different from 1 to 9.
 - By decomposing an audio waveform into frequency contents, we understand what makes the sound of "yes" different from "no"

Determinant

- Given a square matrix $A \in \mathbb{R}^{n \times n}$, the determinant is $det(A) \in \mathbb{R}$
- Use of det(A)
 - Determining the inverse of A
 - Determining singularity (or invertibility) of A

$$det(\mathbf{A}) = |\mathbf{A}| = \begin{vmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{vmatrix} \in \mathbb{R}$$

Determinant of $A \in \mathbb{R}^{1 \times 1}$

$$det(A) = |a_{11}| = a_{11}$$

Determinant of $A \in \mathbb{R}^{2 \times 2}$

$$det(\mathbf{A}) = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

Determinant of $A \in \mathbb{R}^{3\times3}$

$$det(A) = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix}$$

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

 $\pmb{A} \in \mathbb{R}^{3 imes 3}$ can be computed by breaking it down into determinants of $\pmb{A}_i \in \mathbb{R}^{2 imes 2}$

Color coding shows computation of first term using a_{11} $\begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix}$

The coefficient of each term is multiplied by $(-1)^{ij}$. For example, the coefficient of a_{12} is $(-1)^{12} = -1$ This method is known as **Laplace Expansion**

Determinant of $A \in \mathbb{R}^{n \times n}$ (Laplace Expansion)

- For $j=1,2,\ldots,n$ and A_{jk} is the sub-matrix left after deleting row j and column k
- Expansion along column *j*:

$$det(\mathbf{A}) = \sum_{k=1}^{n} (-1)^{k+j} a_{kj} det(\mathbf{A}_{kj})$$

• Expansion along row *j*:

$$det(\mathbf{A}) = \sum_{k=1}^{n} (-1)^{k+j} a_{jk} det(\mathbf{A}_{jk})$$

Exercise: What is det(A) if $A \in \mathbb{R}^{4 \times 4}$

$$det(\mathbf{A}) = \begin{vmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{vmatrix}$$

Special Case: Determinant of a Triangular Matrix

Upper Triangular:
$$\mathbf{T} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{12} & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_{(n-1)1} \\ 0 & \cdots & 0 & a_{nn} \end{bmatrix}$$
, $det(\mathbf{T}) = \prod_{i=1}^n a_{ii}$

Lower Triangular:
$$\mathbf{T} = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & 0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ a_{n1} & \cdots & a_{n(n-1)} & a_{nn} \end{bmatrix}$$
, $det(\mathbf{T}) = \prod_{i=1}^n a_{ii}$

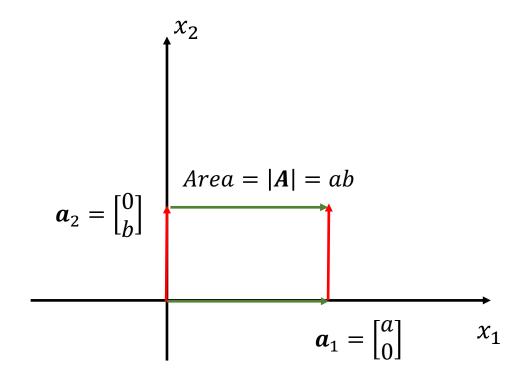
• Consider a > 0 and b > 0:

$$\mathbf{A} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 \end{bmatrix}$$

• Determinant:

$$|A| = ab$$

The Area = |det(A)| holds true even for non-canonical vectors

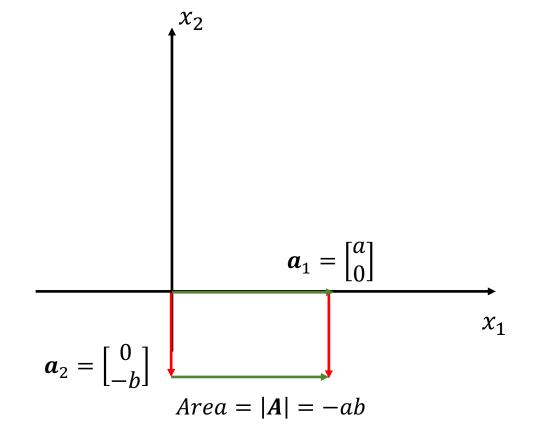


• Consider a > 0 and b > 0:

$$\mathbf{A} = \begin{bmatrix} a & 0 \\ 0 & -h \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 \end{bmatrix}$$

• Determinant:

$$|A| = -ab$$



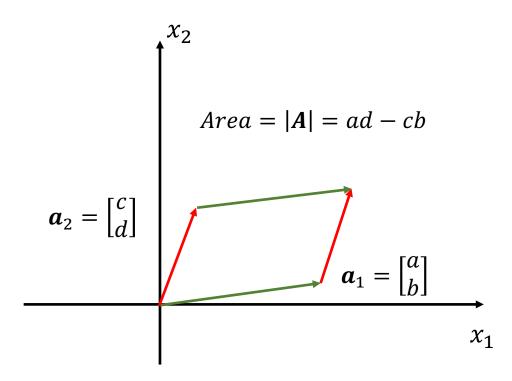
• Consider:

$$\mathbf{A} = \begin{bmatrix} a & c \\ b & d \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 \end{bmatrix}$$

• Determinant:

$$|A| = ad - cb$$

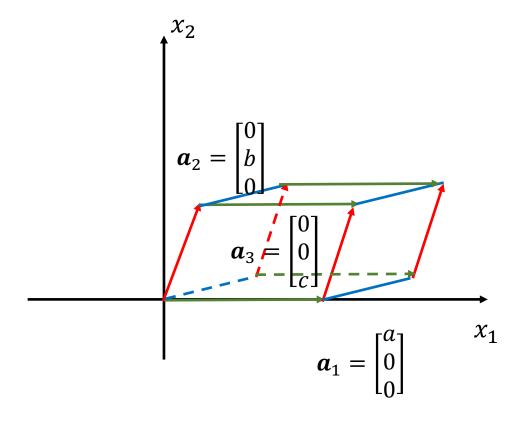
- Exercise:
 - Using trigonometric identities, prove that the area of the parallelogram is |A| = ad cb



• Consider a > 0 , b > 0, c > 0:

$$\mathbf{A} = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 & \mathbf{a}_3 \end{bmatrix}$$

- Determinant: $Signed\ Volume = |A| = abc$
- The Volume = |det(A)| holds true even for non-canonical vectors



$$Vol = |A| = abc$$

Properties of det(A) of $A \in \mathbb{R}^{n \times n}$

- det(AB) = det(A) det(B)
- $det(A) = det(A^T)$
- If A is invertible, $det(A^{-1}) = \frac{1}{det(A)}$
- Similar matrices have the same determinant,
 - $det(\Phi(A)) = det(A)$

- Adding a multiple of a row/col to another does not change the determinant det(A)
- Multiplication of A by $\lambda \in \mathbb{R}$ scales the determinant by λ :
 - $det(\lambda A) = \lambda^n det(A)$
- Swapping row/col of A changes the sign of det(A)

Numerical Method in Determining Determinant

- Using the properties in the red box (previous slide):
 - Use Gaussian Elimination to reduce the matrix into upper triangular form
 - Use property $det(T) = \prod_{i=1}^{n} a_{ii}$ to compute the determinant

Example

Determinant and Rank of $\mathbf{A} \in \mathbb{R}^{n \times n}$

• If $det(A) \neq 0$, then rank(A) = n

Trace

Trace of $A \in \mathbb{R}^{n \times n}$

• Trace of *A* is the sum of its diagonal elements:

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

Properties of Trace of $A, B, I \in \mathbb{R}^{n \times n}$

- tr(A + B) = tr(A) + tr(B)
- $tr(\alpha A) = \alpha tr(A), \alpha \in \mathbb{R}$
- tr(I) = n
- tr(AB) = tr(BA)
 - $A \in \mathbb{R}^{n \times k}$, $B \in \mathbb{R}^{k \times n}$
- tr(AKL) = tr(KLA)
 - $A \in \mathbb{R}^{a \times k}$, $K \in \mathbb{R}^{k \times l}$, $L \in \mathbb{R}^{l \times a}$
- $tr(\mathbf{x}\mathbf{y}^T) = tr(\mathbf{y}^T\mathbf{x}) = \mathbf{y}^T\mathbf{x} \in \mathbb{R}$

Properties of Trace

- Let $\Phi: V \to V$ be a linear mapping
 - If A is used to represent the transformation, then $tr(\Phi) = tr(A)$
 - If B is used to represent the transformation on another basis, then $tr(\Phi) = tr(B) = tr(S^{-1}AS) = tr(ASS^{-1}) = tr(A)$
 - $: tr(\Phi)$ is basis independent

Characteristic Polynomial

• Given $A \in \mathbb{R}^{n \times n}$ and $\lambda \in \mathbb{R}$

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

- c_0 , c_1 , c_2 , ..., c_{n-1} are characteristic polynomial of \boldsymbol{A}
- $c_0 = det(A)$
- $c_{n-1} = (-1)^{n-1} tr(A)$

Eigenvalue and Eigenvectors

Eigenvalue and Eigenvectors

- Certain vectors respond to certain transformation matrices in such a way that the effect is just a constant scaling
- Let $A \in \mathbb{R}^{n \times n}$ and $\lambda \in \mathbb{R}$. $x \in \mathbb{R}^n \setminus \{0\}$ is an eigenvector of A while λ is the corresponding eigenvalue if:

$$Ax = \lambda x$$

Properties of Eigenvalue and Eigenvector

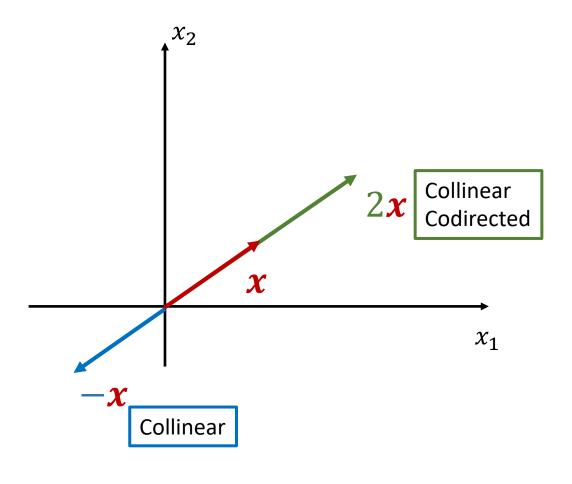
- There exists an $x \in \mathbb{R}^n \setminus \{0\}$ such that $Ax = \lambda x$ for $A \in \mathbb{R}^{n \times n}$ and $\lambda \in \mathbb{R}$ or equivalently $(A \lambda)x = 0$ can be solved with $x \neq 0$
- $rank(A \lambda) < n$
- $det(A \lambda) = 0$

Properties of Eigenvalue and Eigenvector

- Collinear 2 vectors are on the same or opposite direction
- Codirected 2 vectors are on the same direction
- For a given $c \in \mathbb{R} \setminus \{0\}$:

$$Acx = cAx = c\lambda x = \lambda(cx)$$

 \therefore all vectors collinear to x are also eigenvectors



Properties of Eigenvalue and Eigenvector

• λ is an eigenvalue of A if and only if λ is a root of characteristic polynomial of A:

$$p_{A}(\lambda) = det(A - \lambda I) = c_0 + c_1 \lambda + c_2 \lambda^2 + \dots + c_{n-1} \lambda^{n-1} + (-1)^n \lambda^n = 0$$

• The algebraic multiplicity of λ as an eigenvalue of A is the number of times it appears as a root in $p_A(\lambda)$

Eigenspace and Eigenspectrum

- Eigenspace: The set of all eigenvectors, $\{x_1, x_2, ..., x_m\}$ of $A \in \mathbb{R}^{n \times n}$ for a corresponding eigenvalue $\lambda \in \mathbb{R}$ spans a subspace of \mathbb{R}^n called Eigenspace of E_{λ}
- Eigenspectrum: The set of all eigenvalues, $\{\lambda_1, \lambda_2, ..., \lambda_m\}$, of $A \in \mathbb{R}^{n \times n}$
- Identity Matrix $I \in \mathbb{R}^{n \times n}$ has $p_A(\lambda) = det(I \lambda I) = (1 \lambda)^n = 0$
 - Solution is λ repeated n times resulting to Eigenspectrum of $\{1\}$ and Eigenspace $E_{\lambda} = \mathbf{x} \in \mathbb{R}^n$

Other Properties

- The matrix $A \in \mathbb{R}^{n \times n}$ and its transpose $A^T \in \mathbb{R}^{n \times n}$ have the same eigenvalues but not necessarily the same eigenvectors
- Null space or Kernel: The Eigenspace is the Null space or Kernel of $(A \lambda I)$ since $(A \lambda I)x = 0$ or $x \in kernel(A \lambda I)$
- Similar matrices have the same eigenvalues. Therefore, under basis change, the following are invariant:
 - Determinant
 - Trace
 - Eigenvalues
- Positive definite matrices always have positive real eigenvalues

Multiplicity

- The algebraic multiplicity of λ as an eigenvalue of A is the number of times it appears as a root in $p_A(\lambda)$
- The **geometric multiplicity** of λ is the number of independent eigenvectors associated with λ
 - The dimensionality of space spanned by the eigenvectors of λ

Example

- $A = \begin{bmatrix} 2 & 1 \\ 0 & 2 \end{bmatrix}$, solve for the eigenvalues and eigenvectors
- $det(\mathbf{A} \lambda \mathbf{I}) = \begin{bmatrix} 2 \lambda & 1 \\ 0 & 2 \lambda \end{bmatrix} = 0 \Rightarrow p_{\mathbf{A}}(\lambda) = (2 \lambda)(2 \lambda) = 0$
- Eigenvalues: $\lambda_1 = \lambda_2 = 2$, the algebraic multiplicity is 2
- Eigenvectors for : $\lambda_1 = \lambda_2 = 2$
 - $\cdot \begin{bmatrix} 2-2 & 1 \\ 0 & 2-2 \end{bmatrix} x = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} x = \mathbf{0}$
 - $x = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, the geometric multiplicity is 1

Eigenvalues and Eigenvectors of Transformation Matrices

Jupyter Notebook:

More Properties

- Theorem: The eigenvectors $\{x_1, x_2, ..., x_n\}$ of matrix $A \in \mathbb{R}^{n \times n}$ with distinct eigenvalues $\{\lambda_1, \lambda_2, ..., \lambda_n\}$ are linearly independent
 - Definition: If there are fewer than n linearly independent eigenvectors, the matrix is called defective
- Theorem (SPSD): For a given matrix $A \in \mathbb{R}^{n \times n}$, we can always obtain a symmetric positive semi-definite matrix $S \in \mathbb{R}^{n \times n}$: $S = A^T A$
 - If rank(A) = n, then **S** is a symmetric positive definite (SPD) matrix
- Theorem (Spectral Theorem): If $A \in \mathbb{R}^{n \times n}$ is symmetric, there exists an orthonormal basis of vector space V from the eigenvectors of A and each eigenvalue is real.

Determinant and Eigenvalues

• Theorem: The determinant of matrix $A \in \mathbb{R}^{n \times n}$ is the product of its eigenvalues:

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

where $\lambda_i \in \mathbb{C}$ (complex) and may be repeated eigenvalues of A

Trace and Eigenvalues

• Theorem: The trace of matrix $A \in \mathbb{R}^{n \times n}$ is the sum of its eigenvalues:

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

where $\lambda_i \in \mathbb{C}$ (complex) and may be repeated eigenvalues of A

Cholesky Decomposition

Decomposition as Product of 2 Numbers

- In positive real numbers, square root of a number is a useful decomposition. A number is expressed as a product of 2 identical numbers.
 - The square root of area of square is the length of its side: $A = s^2$
 - The square root of a number greater than 1 is always greater than 1:
 - $n = m^2, n, m > 1$
 - The square root of a number less than 1 is always less than 1
 - $n = m^2, n, m < 1$
- In positive integers, factorization determines if a number is prime.
 - A number is prime if it has only 2 factors: itself and 1
- Can we factor $A \in \mathbb{R}^{n \times n}$ as a product of 2 matrices (not exactly identical)?

Cholesky Decomposition

• Theorem: A symmetric positive definite matrix $A \in \mathbb{R}^{n \times n}$ can be decomposed into a product of 2 matrices $A = LL^T$ where L is a lower triangular matrix with positive diagonal elements:

$$\mathbf{A} = \begin{bmatrix} a_{11} & \dots & a_{n1} \\ \vdots & \ddots & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ l_{n1} & \dots & l_{nn} \end{bmatrix} \begin{bmatrix} l_{11} & \dots & l_{n1} \\ \vdots & \ddots & \vdots \\ 0 & \dots & l_{nn} \end{bmatrix}$$

• L is called the Cholesky factor of A and it is unique

Example Cholesky Decomposition

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} & l_{31} \\ 0 & l_{22} & l_{32} \\ 0 & 0 & l_{33} \end{bmatrix}$$

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

Example Cholesky Decomposition

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

•
$$l_{11} = \sqrt{a_{11}}$$

•
$$l_{21} = \frac{a_{21}}{l_{11}}$$

•
$$l_{31} = \frac{a_{31}}{l_{11}}$$

•
$$l_{31} = \frac{a_{31}}{l_{11}}$$

• $l_{22} = \sqrt{a_{22} - l_{21}^2}$

•
$$l_{32} = \frac{a_{32} - l_{21} l_{31}}{l_{32}}$$

•
$$l_{32} = \frac{a_{32} - l_{21} l_{31}}{l_{22}}$$

• $l_{33} = \sqrt{a_{33} - l_{31}^2 - l_{32}^2}$

Cholesky Decomposition: Applications

• Numerical computation of determinant of $A \in \mathbb{R}^{n \times n}$:

$$det(\mathbf{A}) = det(\mathbf{L})det(\mathbf{L}^{T}) = \prod_{i=1}^{n} l_{ii}^{2}$$

 Modelling of covariance matrix of a multi-variate Gaussian which is symmetric and positive definite

Eigendecomposition and Diagonalization

Diagonal Matrices

Determinant, Inverse, and Power are easy to compute for diagonal matrices

• Definition: Diagonal Matrix

$$\mathbf{D} = \begin{bmatrix} d_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & d_{nn} \end{bmatrix}$$

Determinant

$$det(\mathbf{D}) = \prod_{i=1}^{n} d_{ii}$$

Inverse

$$\mathbf{D}^{-1} = \begin{bmatrix} \frac{1}{d_{11}} & \dots & 0\\ \vdots & \ddots & \vdots\\ 0 & \dots & \frac{1}{d_{nn}} \end{bmatrix}$$

Power

$$\boldsymbol{D}^k = \begin{bmatrix} d_{11}^k & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & d_{nn}^k \end{bmatrix}$$

Diagonal Matrices

- Trick: Transform a matrix into a diagonal matrix using change of basis
- Definition (Diagonalizable): A matrix $A \in \mathbb{R}^{n \times n}$ is diagonalizable if it is similar to a diagonal matrix. There exists an invertible matrix $P \in \mathbb{R}^{n \times n}$ such that $D = P^{-1}AP$

The Matrix $P \in \mathbb{R}^{n \times n}$

- Let $\{\lambda_1, \lambda_2, \dots, \lambda_n\}$ be the eigenvalues of matrix $A \in \mathbb{R}^{n \times n}$
- Let $\mathbf{D} = \begin{bmatrix} \lambda_1 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_n \end{bmatrix}$
- Let $oldsymbol{P} = [oldsymbol{p}_1 \quad \cdots \quad oldsymbol{p}_n]$
- Then $m{P}m{D} = m{A}m{P} \Longrightarrow [m{p}_1 \quad \cdots \quad m{p}_n] egin{bmatrix} \lambda_1 & ... & 0 \ dots & \ddots & dots \ 0 & ... & \lambda_n \end{bmatrix} = m{A}[m{p}_1 \quad \cdots \quad m{p}_n]$
- $\lambda_1 \boldsymbol{p}_1 = A \boldsymbol{p}_1$, ..., $\lambda_n \boldsymbol{p}_n = A \boldsymbol{p}_n$
- p_1 , ..., p_n are eigenvectors of A that must linearly independent so that P is invertible

Eigendecomposition

• Theorem (Eigendecomposition): A square matrix $A \in \mathbb{R}^{n \times n}$ can be factored into:

$$A = PDP^{-1}$$

Where

$$m{D} = egin{bmatrix} \lambda_1 & \dots & 0 \ dots & \ddots & dots \ 0 & \dots & \lambda_n \end{bmatrix}$$
 and $m{P} = [m{p}_1 & \cdots & m{p}_n]$ are linearly independent

eigenvectors of \hat{A} or the basis of \mathbb{R}^n

Example

- Given $A = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$, perform Eigendecomposition
- Let $\mathbf{D} = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}$
- Let $oldsymbol{P} = [oldsymbol{p}_1 \quad oldsymbol{p}_2]$
- To find the eigenvalues: $det(A \lambda I) = \begin{vmatrix} \frac{5}{2} \lambda & -1 \\ -1 & \frac{5}{2} \lambda \end{vmatrix} = \mathbf{0}$
- The characteristic polynomial:

•
$$\left(\frac{5}{2} - \lambda\right)^2 - 1 = 0 \text{ or } \lambda = \frac{7}{2}, \frac{3}{2}$$

$$\bullet \therefore \mathbf{D} = \begin{bmatrix} \frac{7}{2} & 0 \\ 0 & \frac{3}{2} \end{bmatrix}$$

•
$$A\mathbf{p}_1 = \lambda_1 \mathbf{p}_1 \implies \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix} \mathbf{p}_1 = \frac{7}{2} \mathbf{p}_1 \implies \begin{bmatrix} 5 - 7 & -2 \\ -2 & 5 - 7 \end{bmatrix} \mathbf{p}_1$$

•
$$\Rightarrow \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \boldsymbol{p}_1 \Rightarrow \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \boldsymbol{p}_1 \text{ by GE or } \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix} \boldsymbol{p}_1 \text{ by } -1 \text{ Trick}$$

•
$$p_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$
, similarly $p_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$ or $P = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$, $P^{-1} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$

Check

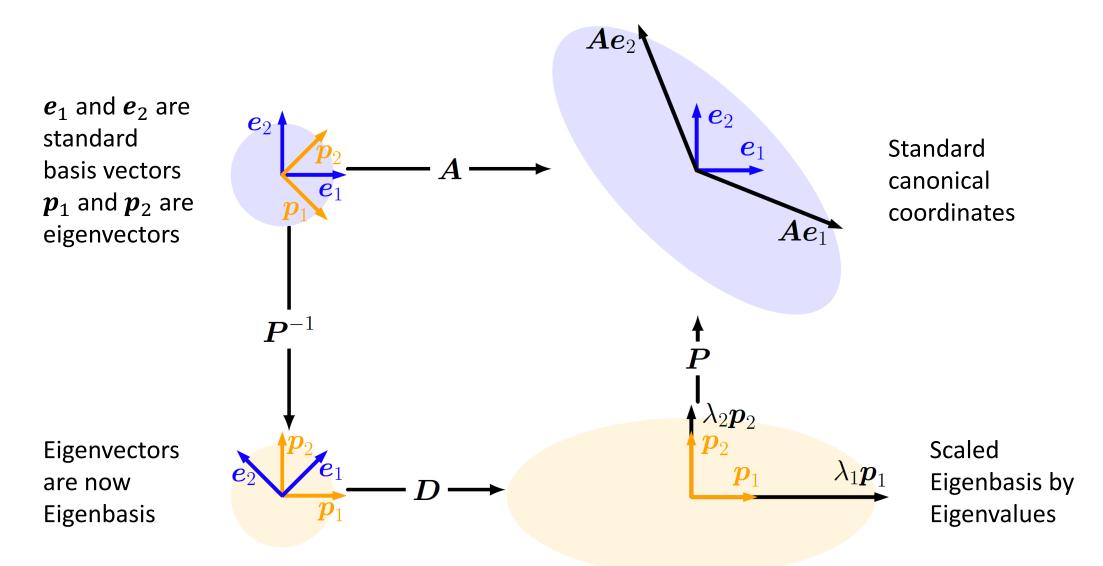
•
$$A = PDP^{-1} = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \frac{7}{2} & 0 \\ 0 & \frac{3}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{7}{2} & \frac{3}{2} \\ \frac{7}{2} & \frac{3}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

$$\bullet \mathbf{A} = \frac{1}{2} \begin{bmatrix} 5 & -2 \\ -2 & 5 \end{bmatrix}$$

Symmetric Matrix

- Theorem (Eigendecomposition of Symmetric Matrix): A symmetric matrix $S \in \mathbb{R}^{n \times n}$ can always be diagonalized
- Proof: A symmetric matrix has an orthonormal eigenvectors
- *Implication*: **P** is an orthogonal matrix

Geometric Interpretation



Benefits of Eigendecomposition

- Power: $A^k = (PDP^{-1})^k = PD^kP^{-1}$
- $det(\mathbf{A}) = det(\mathbf{P}\mathbf{D}\mathbf{P}^{-1}) = det(\mathbf{P})det(\mathbf{D})det(\mathbf{P}^{-1})$
- $\Rightarrow det(\mathbf{P}) \prod_{i=1}^{n} d_{ii} det(\mathbf{P}^{-1}) = \prod_{i=1}^{n} d_{ii} det(\mathbf{P}) det(\mathbf{P}^{-1})$
- $\Rightarrow \prod_{i=1}^{n} d_{ii} PP^{-1} = \prod_{i=1}^{n} d_{ii} = \prod_{i=1}^{n} \lambda_{i}$

Singular Value Decomposition

Singular Value Decomposition (SVD)

- Eigendecomposition and Cholesky Decomposition are limited to square matrices
- SVD exists for all matrices

SVD

• Theorem (SVD): Let $A \in \mathbb{R}^{m \times n}$ be a rectangular matrix of rank $r \in [0, \min(m, n)]$. The SVD of A is a decomposition of the form:

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} = \begin{bmatrix} u_{11} & \dots & u_{1m} \\ \vdots & \ddots & \vdots \\ u_{m1} & \dots & u_{mm} \end{bmatrix} \begin{bmatrix} \sigma_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{mn} \end{bmatrix} \begin{bmatrix} v_{11} & \dots & v_{1n} \\ \vdots & \ddots & \vdots \\ v_{n1} & \dots & v_{nn} \end{bmatrix}^T$$

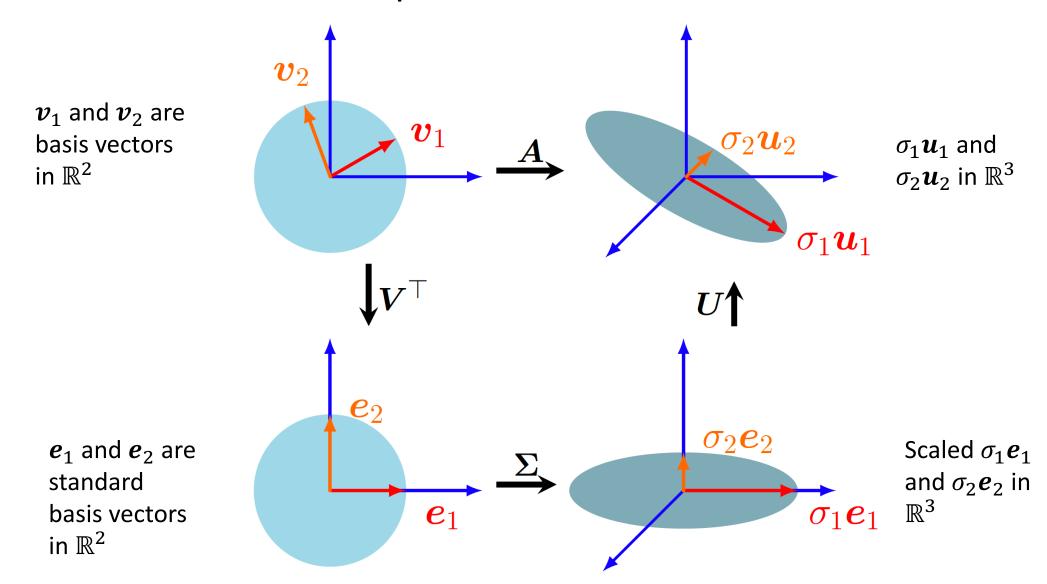
$$[\boldsymbol{a}_1 \quad \cdots \quad \boldsymbol{a}_n] = [\boldsymbol{u}_1 \quad \cdots \quad \boldsymbol{u}_m][\boldsymbol{\sigma}_1 \quad \cdots \quad \boldsymbol{\sigma}_n][\boldsymbol{v}_1 \quad \cdots \quad \boldsymbol{v}_n]^T$$

- Orthogonal matrix: $\mathbf{U} \in \mathbb{R}^{m \times m}$, $\mathbf{\Sigma} \in \mathbb{R}^{m \times n}$, Orthogonal matrix: $\mathbf{V} \in \mathbb{R}^{n \times n}$
- $\sigma_{ii} \geq 0$ (singular values), $\sigma_{ij} = 0$ for $i \neq j$

SVD

- u_i left singular vectors
- v_i right singular vectors

Geometric Interpretation



Example

• Jupyter Notebook:

• Consider the Eigendecomposition of a Symmetric Positive Definite (SPD) matrix:

$$S = S^T = PDP^T$$

• This is similar in form to:

$$S = U\Sigma V^T$$

• In other words, the SVD of an SPD is an Eigendecomposition of ${m S}={m S}^T$

- Given $A \in \mathbb{R}^{m \times n}$, then $S = A^T A$ is a symmetric positive semi-definite matrix by SPSD Theorem
- By *Spectral Theorem*, there exists an orthonormal basis and *S* can be diagonalized.

$$S = A^{T}A = PDP^{T} = P\begin{bmatrix} \lambda_{1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \lambda_{n} \end{bmatrix} P^{T}$$

• P is an orthogonal matrix made of orthonormal eigen basis

• Assume that the SVD of $A = U\Sigma V^T$ exists, then:

$$A^{T}A = (U\Sigma V^{T})^{T}U\Sigma V^{T} = V\Sigma^{T}U^{T}U\Sigma V^{T} = V\Sigma^{T}\Sigma V^{T}$$

• Since $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$

$$\mathbf{A}^T \mathbf{A} = \mathbf{V} \begin{vmatrix} \sigma_1^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_n^2 \end{vmatrix} \mathbf{V}^T$$

• :: P = V and $\lambda_i = \sigma_i^2$

• To obtain U, we use the same procedure except we compute for:

$$AA^{T} = U\Sigma V^{T}(U\Sigma V^{T})^{T} = U\Sigma^{T}V^{T}V\Sigma U^{T} = U\Sigma^{T}\Sigma U^{T}$$

• Since $V^TV = I$

$$AA^T = U \begin{bmatrix} \sigma_1^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_n^2 \end{bmatrix} U^T$$

• :: P = U and $\lambda_i = \sigma_i^2$

SVD Algorithm – Connecting $oldsymbol{U}$ and $oldsymbol{V}$

• Since the columns of V are orthonormal, for $i \neq j$:

$$(Av_i)^T A v_j = 0$$

$$(\mathbf{A}v_i)^T \mathbf{A}v_j = v_i^T \mathbf{A}^T \mathbf{A}v_j = v_i^T \sigma_i \sigma_j v_j = \sigma_i \sigma_j v_i^T v_j = 0$$

SVD Algorithm – Connecting $oldsymbol{U}$ and $oldsymbol{V}$

• Since the columns of V are orthonormal, for $i \neq j$:

$$(A\boldsymbol{v}_i)^T A\boldsymbol{v}_j = 0$$

$$(\mathbf{A}\boldsymbol{v}_i)^T \mathbf{A}\boldsymbol{v}_j = \boldsymbol{v}_i^T \mathbf{A}^T \mathbf{A}\boldsymbol{v}_j = \boldsymbol{v}_i^T \sigma_i \sigma_j \boldsymbol{v}_j = \sigma_i \sigma_j \boldsymbol{v}_i^T \boldsymbol{v}_j = 0$$

• For *i*:

$$(\mathbf{A}\mathbf{v}_i)^T \mathbf{A}\mathbf{v}_i = \sigma_i^2 \mathbf{v}_i^T \mathbf{v}_i \Rightarrow \|\mathbf{A}\mathbf{v}_i\| = \sigma_i \|\mathbf{v}_i\| = \sigma_i \sqrt{\mathbf{v}_i^T \mathbf{v}_i} = \sigma_i$$

• Furthermore,

$$\boldsymbol{u}_i = \frac{A\boldsymbol{v}_i}{\|A\boldsymbol{v}_i\|} = \frac{1}{\sigma_i}A\boldsymbol{v}_i$$

SVD Algorithm – Connecting $oldsymbol{U}$ and $oldsymbol{V}$

Therefore,

$$Av_i = \sigma_i u_i = u_i \sigma_i$$

- The above equation holds for i = 1, ..., r where $r = \min(m, n)$
- If m>n=r, we know that for i>r, $Av_i=\mathbf{0}$
- If r = m < n, we know that for i > r, u_i vectors are orthonormal
- Therefore,

$$AV = U\Sigma \Rightarrow A = U\Sigma V^T$$

• Since for orthogonal matrix: $V^{-1} = V^T$

Example: Perform SVD on
$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 1 \end{bmatrix}$$

• We need to solve for Σ and V: $A^TA = V\Sigma^T\Sigma V^T$

•
$$A^T A = \begin{bmatrix} 1 & -1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}$$

• The diagonal elements of $\mathbf{\Sigma}^T\mathbf{\Sigma}$ are the Eigenvalues of $\mathbf{A}^T\mathbf{A}$

•
$$det(A - \lambda I) = \begin{bmatrix} 2 - \lambda & -1 \\ -1 & 2 - \lambda \end{bmatrix} = 0, \lambda_1 = \sigma_1^2 = 3, \lambda_2 = \sigma_2^2 = 1$$

•
$$\mathbf{\Sigma} = \begin{bmatrix} \sigma_1 & 0 & 0 \\ 0 & \sigma_2 & 0 \end{bmatrix} = \begin{bmatrix} \sqrt{3} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

•
$$A^T A v_1 = \lambda_1 v_1 \Longrightarrow \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} v_1 = 3I v_1 \Longrightarrow v_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Example: Perform SVD on $\mathbf{A} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 1 \end{bmatrix}$

•
$$A^T A v_2 = \lambda_2 v_2 \Longrightarrow \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix} v_2 = I v_2 \Longrightarrow v_2 = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

•
$$\mathbf{V} = \begin{bmatrix} \mathbf{v}_1 & \mathbf{v}_2 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix} \Longrightarrow \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

• Solving for *U*:

•
$$u_1 = \frac{Av_1}{\sigma_1} = \frac{\begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}}{\sqrt{3}} = \begin{bmatrix} \frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \end{bmatrix}$$
, $u_2 = \frac{Av_2}{\sigma_2} = \frac{\begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}}{1} = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{bmatrix}$

Example: Perform SVD on
$$\mathbf{A} = \begin{bmatrix} 1 & 0 \\ -1 & 1 \\ 0 & 1 \end{bmatrix}$$

• Solving for *U*:

•
$$u_3 = u_1 \times u_2 = \begin{bmatrix} \frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \end{bmatrix} \times \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{bmatrix}$$

•
$$\mathbf{U} = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} \\ -\frac{2}{\sqrt{6}} & 0 & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{6}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{3}} \end{bmatrix}$$

Eigendecomposition vs SVD

$$A = PDP^{-1}$$

- Exists for square matrix $A \in \mathbb{R}^{n \times n}$ with basis eigenvectors of \mathbb{R}^n
- P vectors are not necessarily orthogonal. Hence, may not represent rotations

$$A = U\Sigma V^T$$

- Exists for any matrix $A \in \mathbb{R}^{m \times n}$
- U and V^T vectors are orthonormal. Hence, they represent rotations

Eigendecomposition vs SVD

$$A = PDP^{-1}$$

- Linear Mapping
 - Change of basis in the domain
 - Independent scaling of new basis.
 Mapping from domain to codomain.
 - Change of basis in the codomain
- Domain and codomain must have the same dimension

$$A = U\Sigma V^T$$

- Linear Mapping
 - Change of basis in the domain
 - Independent scaling of new basis.
 Mapping from domain to codomain.
 - Change of basis in the codomain
- Domain and codomain may have different dimensions

Eigendecomposition vs SVD

$$A = PDP^{-1}$$

- P and P^{-1} are inverses of each other
- **D** : real or complex eigenvalues
- If A is symmetric, the Eigendecomposition is equal to SVD

$$A = U\Sigma V^T$$

- U and V are not necessarily inverses of each other
- Σ : the non-zero entries are real and positive
- Σ : the non-zero eigenvalues are square root of non-zero eigenvalues of A^TA which are equal to non-zero eigenvalues of A^TA
- If A is symmetric, the SVD is equal to Eigendecomposition

Matrix Approximation

Low-Rank Approximation of $A \in \mathbb{R}^{m \times n}$

- Assume SVD: $A = U\Sigma V^T$
- ullet Assume the singular values in $oldsymbol{\Sigma}$ are sorted in descending order
- Rank 1 approximation of *A*:

$$\boldsymbol{A} \approx \sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1^T$$

• Rank 2 approximation of *A*:

$$\boldsymbol{A} \approx \sigma_1 \boldsymbol{u}_1 \boldsymbol{v}_1^T + \sigma_2 \boldsymbol{u}_2 \boldsymbol{v}_2^T$$

• Rank k (where $k \le r = number$ of non - zero singular values) approximation of A:

$$A \approx \widehat{A}(k) = \sum_{i=1}^k \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T$$

Application of Low-Rank Approximation

- For example, given a 640×480 grayscale image. The total number to represent the image is 307,200
- A rank 3 approximation is only $3\times(640+480)=3,360$ which is just 1% of the original size

Distance/Norm of Low-Rank Approximation

- Given $A \in \mathbb{R}^{m \times n}$, distance or norm measures how far is the low-rank approximation $\widehat{A}(k)$ from A
- Definition (Spectral Norm of a Matrix): For $x \in \mathbb{R}^n \setminus \{0\}$, the spectral norm of $A \in \mathbb{R}^{m \times n}$ is:

$$||A||_2 := \max_{x} \frac{||Ax||_2}{||x||_2}$$

• Theorem (Spectral Norm): The spectral norm of ${\it A}$ is its largest singular value σ_1 .

Distance/Norm of Low-Rank Approximation

• Theorem (Eckart-Young): Consider a matrix $A \in \mathbb{R}^{m \times n}$ of rank r and any matrix $B \in \mathbb{R}^{m \times n}$ of rank k. For any $k \leq r$ with $\widehat{A}(k) = \sum_{i=1}^k \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T$, it holds that:

$$\widehat{A}(k) = \operatorname{argmin}_{rank(B)=k} ||A - B||_2,$$

$$\|\mathbf{A} - \widehat{\mathbf{A}}(k)\|_2 = \sigma_{k+1}$$

Eckart-Young Theorem

• We can justify $\| \boldsymbol{A} - \widehat{\boldsymbol{A}}(k) \|_2 = \sigma_{k+1}$ since:

$$A - \widehat{A}(k) = \sum_{i=k+1}^{r} \sigma_i \boldsymbol{u}_i \boldsymbol{v}_i^T$$

• Eckart-Young Theorem shows that $\widehat{A}(k)$ is an optimal low-rank approximation of A

End