## 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 to help us design a better logistic regressor

By decomposing an audio waveform into frequency contents, we understand what makes the sound of "yes" different from "no"

By decomposing connectivity (edges) in a graph neural network, we understand which neurons (nodes) are triggered while an agent is solving a task

#### 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 $A \in \mathbb{R}^{3\times3}$

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

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

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

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  $(-1)^{i+j}$ . For example, the coefficient of  $a_{12}$  is  $(-1)^{1+2}=-1$ 

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: 
$$\mathbf{T} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_{(n-1)1} \\ 0 & \cdots & 0 & a_{nn} \end{bmatrix}$$
,  $det(\mathbf{T}) = \prod_{i=1}^n a_{ii}$ 

Lower Triangular: 
$$\mathbf{T} = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ a_{n1} & \cdots & a_{n(n-1)} & a_{nn} \end{bmatrix}$$
,  $det(\mathbf{T}) = \prod_{i=1}^n a_{ii}$ 

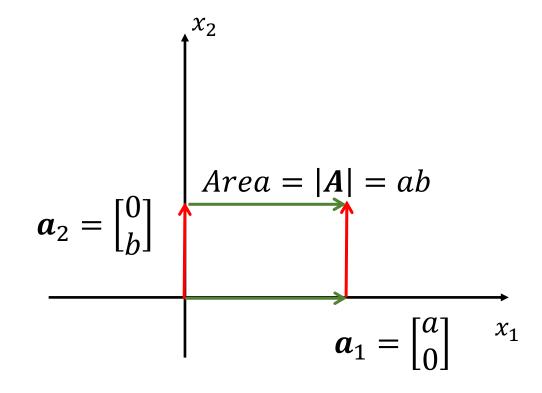
Consider a > 0 and b > 0:

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

**Determinant:** 

$$|A| = ab$$

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

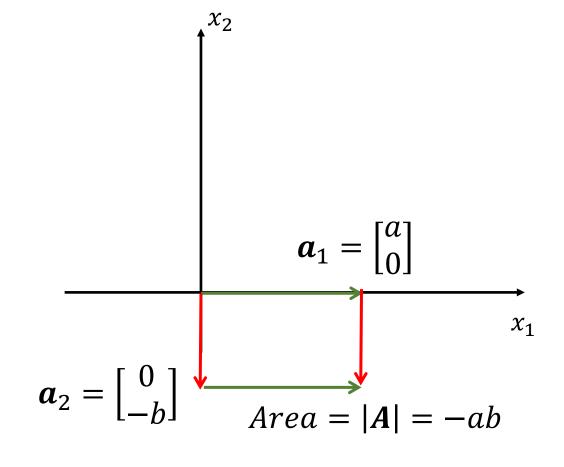


Consider a > 0 and b > 0:

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

**Determinant:** 

$$|A| = -ab$$



#### Consider:

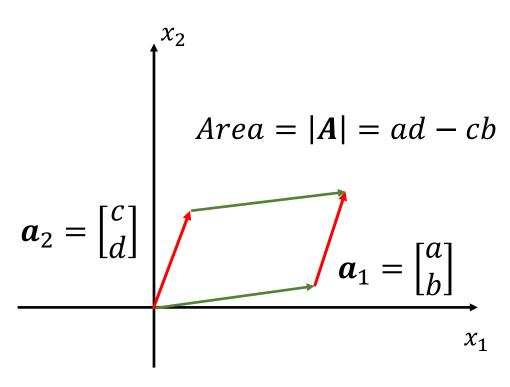
$$\mathbf{A} = \begin{bmatrix} a & c \\ b & d \end{bmatrix} = \begin{bmatrix} \mathbf{a}_1 & \mathbf{a}_2 \end{bmatrix}$$

#### **Determinant:**

$$|A| = ad - cb$$

#### Exercise:

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



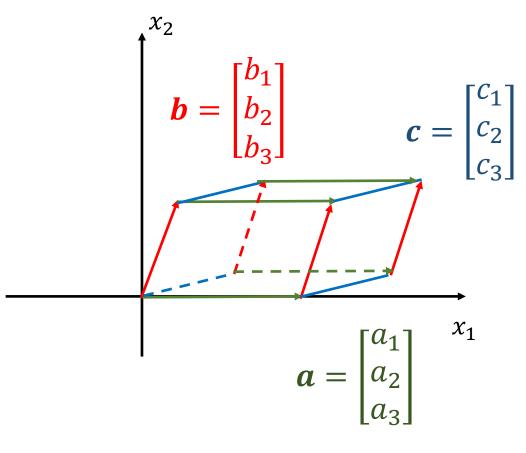
#### Consider:

$$A = \begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix} = [ a \quad b \quad c ]$$

**Determinant:** 

$$Signed\ Volume = det(A) = |A|$$

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



$$Vol = |A|$$

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

det(AB) = det(A) det(B)

$$det(\mathbf{A}) = det(\mathbf{A}^T)$$

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  $\lambda$ :

$$det(\lambda A) = \lambda^n det(A)$$

Swapping row/col of A changes the sign of det(A)

#### Similar Matrices

Two matrices  $A, \widetilde{A} \in \mathbb{R}^{n \times n}$ , there exists a regular matrix  $S \in \mathbb{R}^{n \times n}$  such that:

$$\widetilde{A} = S^{-1}AS$$

$$det(\widetilde{A}) = det(S^{-1}AS) = det(A)det(S^{-1}S) = det(A)$$

# Numerical Method in Determining Determinant

Using the properties in the 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

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & -1 & 1 \\ 0 & 1 & 2 & 0 \\ 2 & 0 & 0 & -1 \\ -1 & 1 & 0 & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & -1 & 1 \\ 0 & 1 & 2 & 0 \\ 0 & 0 & 2 & -3 \\ 0 & 0 & 0 & -1.5 \end{bmatrix}$$

$$det(A) = 1 \cdot 1 \cdot 2 \cdot -1.5 = -3$$

#### 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 $A, B, I \in \mathbb{R}^{n \times n}$

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

#### Properties of Trace

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

## 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  $\lambda$  is the corresponding eigenvalue if:

$$Ax = \lambda x$$

#### Properties of Eigenvalue and Eigenvector

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

### Characteristic Polynomial

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

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

 $c_0, c_1, c_2, \dots, c_{n-1}$  are characteristic polynomial of  $\boldsymbol{A}$ 

$$c_0 = det(A)$$

$$c_{n-1} = (-1)^{n-1} tr(A)$$

#### Non-uniqueness of Eigenvector

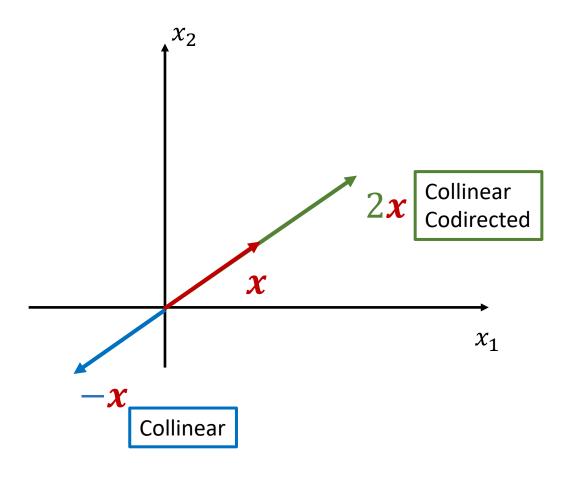
Collinear – 2 vectors are on the same or opposite direction

Codirected – 2 vectors are on the same direction

For a given  $c \in \mathbb{R} \setminus \{0\}$ :

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

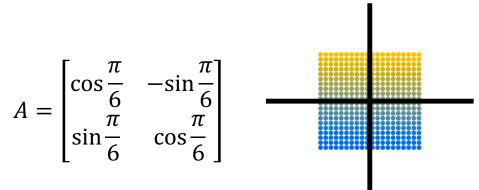
 $\therefore$  all vectors collinear to x are also eigenvectors; same eigenvalue, different eigenvectors

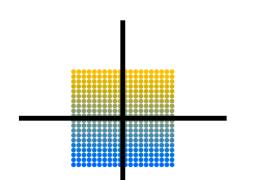


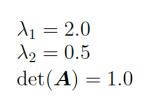
$$A = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{bmatrix}$$

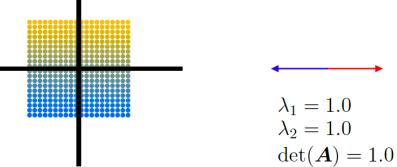
$$A = \begin{bmatrix} 1 & \frac{1}{2} \\ 0 & 1 \end{bmatrix}$$

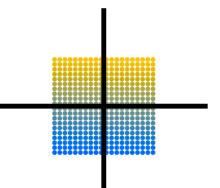
$$\begin{bmatrix} \cos \frac{\pi}{6} \end{bmatrix}$$

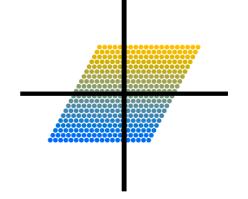


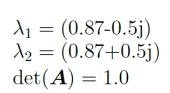










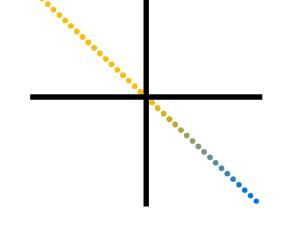


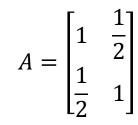
$$A = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

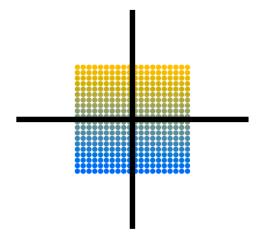
$$\lambda_1 = 0.0$$

$$\lambda_2 = 2.0$$

$$\det(\mathbf{A}) = 0.0$$





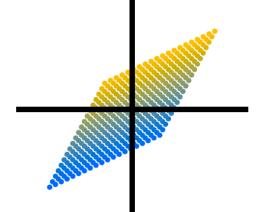




$$\lambda_1 = 0.5$$

$$\lambda_2 = 1.5$$

$$\det(\mathbf{A}) = 0.75$$



#### Properties of Eigenvalue and Eigenvector

 $\lambda$  is an eigenvalue of  $\boldsymbol{A}$  if and only if  $\lambda$  is a root of characteristic polynomial of  $\boldsymbol{A}$ :

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

The algebraic multiplicity of  $\lambda$  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  $E_{\lambda}$ 

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

The **geometric multiplicity** of  $\lambda$  is the number of independent eigenvectors associated with  $\lambda$ 

The dimensionality of space spanned by the eigenvectors of  $\lambda$ 

#### Example

$$A = \begin{bmatrix} 2 & 1 \\ 0 & 2 \end{bmatrix}, \text{ solve for the eigenvalues and eigenvectors}$$
 
$$det(A - \lambda I) = \begin{bmatrix} 2 - \lambda & 1 \\ 0 & 2 - \lambda \end{bmatrix} = 0 \Rightarrow p_A(\lambda) = (2 - \lambda)(2 - \lambda) = 0$$
 
$$det(A - \lambda I) = 4 - 4\lambda + \lambda^2, det(A) = 4, -4 = -1^1 Tr(A),$$
 Eigenvalues:  $\lambda_1 = \lambda_2 = 2$ , the algebraic multiplicity is 2 Eigenvectors for:  $\lambda_1 = \lambda_2 = 2$  
$$\begin{bmatrix} 2 - 2 & 1 \\ 0 & 2 - 2 \end{bmatrix} x = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} x = 0$$
 
$$x = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \text{ the geometric multiplicity is 1}$$

#### Eigenvalues and Eigenvectors

```
>>> import numpy as np
>>> a = np.array([[2, 1],[0, 2]])
>>> a.shape
(2, 2)
>>> np.linalg.det(a)
4.0
>>> np.linalg.eig(a)
(array([2., 2.]), array([[ 1.0000000e+00, -1.0000000e+00],
       [0.0000000e+00, 4.4408921e-16]])
>>>
```

### Recall: Symmetric Positive Definite Matrix

Symmetric Positive Definite Matrix implies:

$$\forall x \in V \setminus \{\mathbf{0}\}$$
,  $x^T A x > \mathbf{0}$ 

Symmetric Positive Semi-Definite Matrix if:

$$\forall x \in V \setminus \{\mathbf{0}\}$$
,  $x^T A x \geq \mathbf{0}$ 

#### 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:

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

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 or more matrices?

#### 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

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

$$l_{11} = \sqrt{a_{11}}$$

$$l_{22} = \sqrt{a_{22} - l_{21}^2}$$

$$l_{21} = \frac{a_{21}}{l_{11}}$$

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

$$l_{31} = \frac{a_{31}}{l_{11}}$$

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

#### 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

$$m{D}^k = egin{bmatrix} d_{11}^k & ... & 0 \ dots & \ddots & dots \ 0 & ... & d_{nn}^k \end{bmatrix}$$

#### 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  $D = P^{-1}AP$ 

### 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  $oldsymbol{A}$  or the basis of  $\mathbb{R}^n$ 

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

Let  $\{\lambda_1, \lambda_2, ..., \lambda_n\}$  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 
$$\boldsymbol{P} = [\boldsymbol{p}_1 \quad \cdots \quad \boldsymbol{p}_n]$$

Then 
$$extbf{\emph{PD}} = extbf{\emph{AP}} \Longrightarrow [ extbf{\emph{p}}_1 \quad \cdots \quad extbf{\emph{p}}_n] egin{bmatrix} \lambda_1 & \dots & 0 \ \vdots & \ddots & \vdots \ 0 & \dots & \lambda_n \end{bmatrix} = extbf{\emph{A}}[ extbf{\emph{p}}_1 \quad \cdots \quad extbf{\emph{p}}_n]$$

$$\lambda_1 \boldsymbol{p}_1 = A \boldsymbol{p}_1$$
, ...,  $\lambda_n \boldsymbol{p}_n = A \boldsymbol{p}_n$ 

 $p_1, \dots, p_n$  are eigenvectors of A that must be linearly independent so that P is invertible

#### 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  $\mathbf{P}=[\mathbf{p}_1&\mathbf{p}_2]$ 

Let 
$$P = [P_1 \quad P_2]$$
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:

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

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

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

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

$$p_1 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$
, 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

$$\mathbf{A} = \mathbf{P}\mathbf{D}\mathbf{P}^{-1} = \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \frac{7}{2} & 0 \\ 0 & \frac{3}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{7}{2} & \frac{3}{2} \\ \frac{7}{2} & \frac{3}{2} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$$

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

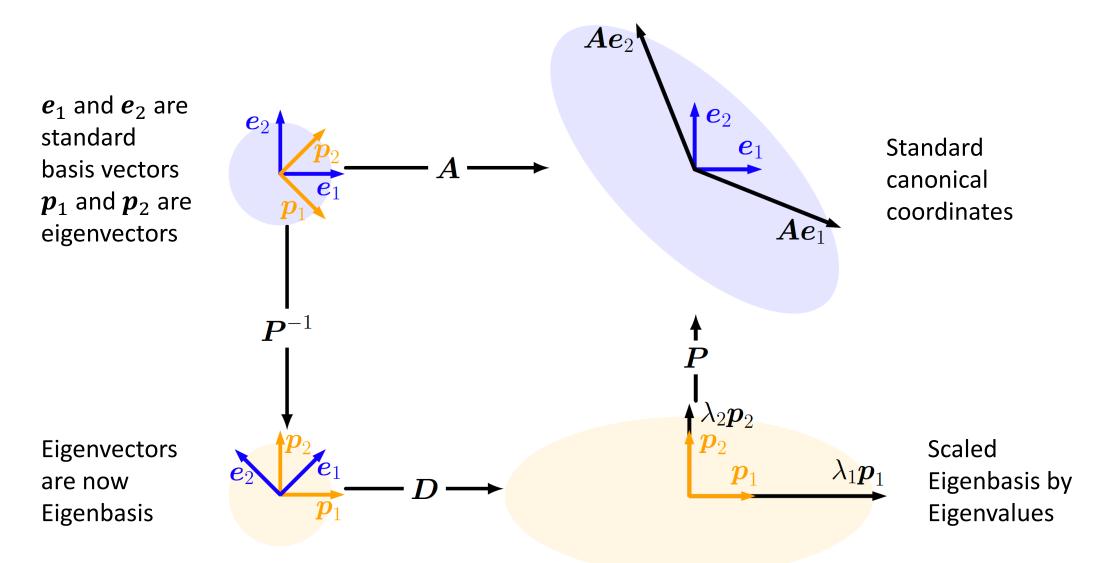
#### Symmetric Matrix

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

# Singular Value Decomposition

#### Singular Value Decomposition (SVD)

Eigendecomposition and Cholesky Decomposition are limited to square matrices

SVD exists for all matrices

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  $\boldsymbol{A}$  is a decomposition of the form:

 $A = U\Sigma V^T$ 

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{m1} & \dots & a_{mn} \end{bmatrix} = \begin{bmatrix} u_{11} & \dots & u_{1m} \\ \vdots & \ddots & \vdots \\ u_{m1} & \dots & u_{mm} \end{bmatrix} \begin{bmatrix} \sigma_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{mn} \end{bmatrix} \begin{bmatrix} v_{11} & \dots & v_{1n} \\ \vdots & \ddots & \vdots \\ v_{n1} & \dots & v_{nn} \end{bmatrix}^T$$
$$[\boldsymbol{a}_1 & \dots & \boldsymbol{a}_n] = [\boldsymbol{u}_1 & \dots & \boldsymbol{u}_m] [\boldsymbol{\sigma}_1 & \dots & \boldsymbol{\sigma}_n] [\boldsymbol{v}_1 & \dots & \boldsymbol{v}_n]^T$$

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

Orthogonal matrix:  $U \in \mathbb{R}^{m \times m}$ , Diagonal Matrix:  $\Sigma \in \mathbb{R}^{m \times n}$ , Orthogonal matrix:  $V \in \mathbb{R}^{m \times n}$  $\mathbb{R}^{n \times n}$ 

 $\sigma_{ii} \geq 0$  (singular values),  $\sigma_{ii} = 0$  for  $i \neq j$ 

#### **SVD**

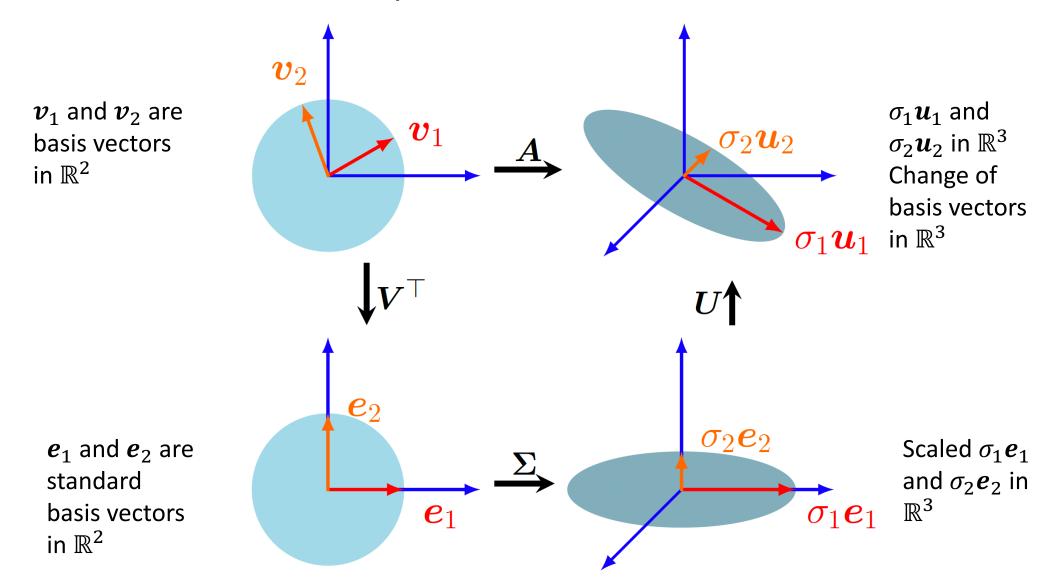
 $oldsymbol{u}_i$ - left singular vectors

 $v_i$ - right singular vectors

 $\Sigma$  – singular matrix

$$\begin{cases} \begin{bmatrix} \sigma_{11} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{nn} \\ 0 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & 0 \end{bmatrix} & if \ m > n \\ \begin{bmatrix} \sigma_{11} & \dots & 0 & 0 & \dots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{mm} & 0 & \dots & 0 \end{bmatrix} & if \ m < n \end{cases}$$

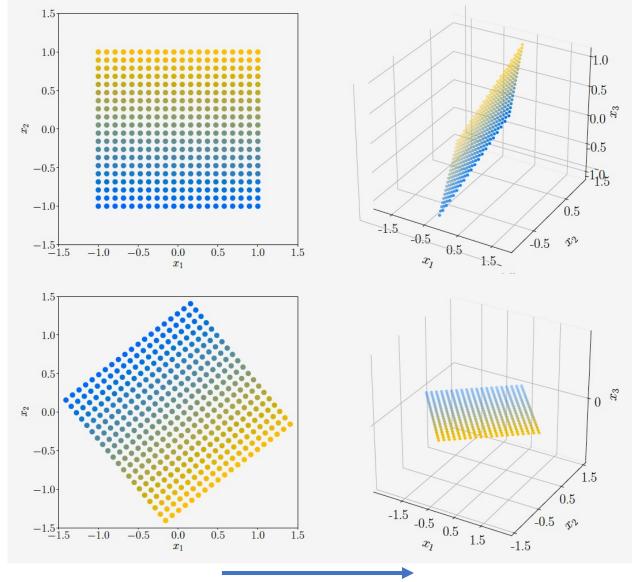
#### Geometric Interpretation



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

#### SVD

Geometric Interpretation





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  $\boldsymbol{S} = \boldsymbol{S}^T$ 

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.

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

 ${m P}$  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  $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$ 

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

$$\therefore \mathbf{P} = \mathbf{V} \text{ and } \lambda_i = \sigma_i^2$$

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  $V^TV = I$ 

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

$$\therefore \mathbf{P} = \mathbf{U} \text{ and } \lambda_i = \sigma_i^2$$

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

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

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

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

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

For *i*:

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

Furthermore,  $AV = U\Sigma \rightarrow Av_i = u_i\sigma_i \ for \ i=1...r$  $u_i$  is simply the normalized image of  $Av_i$ :

$$u_i = \frac{Av_i}{\|Av_i\|} = \frac{1}{\sigma_i}Av_i$$

### 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,  $u_i$  vectors are orthonormal

If r = m < n, we know that for i > r,  $Av_i = 0$ 

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  $\Sigma$  and  $V: A^TA = V\Sigma^T\Sigma V^T$ 

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

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

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

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

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

Solving for *V*:

$$A^{T}Av_{1} = \lambda_{1}v_{1} \Rightarrow \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}v_{1} = 3Iv_{1} \Rightarrow v_{1} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

$$A^{T}Av_{2} = \lambda_{2}v_{2} \Rightarrow \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}v_{2} = Iv_{2} \Rightarrow v_{2} = \begin{bmatrix} -1 \\ -1 \end{bmatrix}$$

$$V = \begin{bmatrix} v_{1} & v_{2} \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ -1 & -1 \end{bmatrix} \Rightarrow \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}$$

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

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 $\mathbf{A} = \begin{bmatrix} 1 & \mathbf{0} \\ -1 & 1 \\ 0 & 1 \end{bmatrix}$

Solving for *U*:

$$\boldsymbol{u}_{3} = \boldsymbol{u}_{1} \times \boldsymbol{u}_{2} = \begin{bmatrix} \frac{1}{\sqrt{6}} \\ -\frac{2}{\sqrt{6}} \\ -\frac{1}{\sqrt{6}} \end{bmatrix} \times \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ -\frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{3}} \end{bmatrix}$$

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

```
>>> a = np.array([[1, 0], [-1, 1], [0, 1]])
>>> a.shape
(3, 2)
>>> np.linalg.svd(a)
(array([-4.08248290e-01, -7.07106781e-01, -5.77350269e-01],
       [ 8.16496581e-01, -5.55111512e-17, -5.77350269e-01],
       [4.08248290e-01, -7.07106781e-01, 5.77350269e-01]]),
array([1.73205081, 1. ]),
array([[-0.70710678, 0.70710678],
       [-0.70710678, -0.70710678]])
>>> np.sqrt(3)
1.7320508075688772
>>> 1/np.sqrt(3)
0.5773502691896258
>>> 1/np.sqrt(6)
0.4082482904638631
>>> 1/np.sqrt(2)
0.7071067811865475
```

### 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

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

 $\boldsymbol{P}$  and  $\boldsymbol{P}^{-1}$  are inverses of each other

 $m{D}$ : real or complex eigenvalues If  $m{A}$  is symmetric, the Eigendecomposition is equal to SVD

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

**U** and **V** are not necessarily inverses of each other

 $\Sigma$ : the non-zero entries are real and positive

 $\Sigma$ : 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  $\boldsymbol{A}$  is symmetric, the SVD is equal to EigenDecomposition

# Matrix Approximation

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

Assume SVD:  $A = U\Sigma V^T$ 

Assume the singular values in  $\Sigma$  are sorted in descending order

Rank 1 approximation of *A*:

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

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

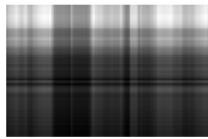
For example, given a  $640 \times 480$  grayscale image. The total number to represent the image is 307,200

A rank 3 approximation is only  $3 \times (640 + 480) + 3 = 3,363$  which is

just 1% of the original size



(a) Original image A.



(b) Rank-1 approximation  $\widehat{A}(1)$ .(c) Rank-2 approximation  $\widehat{A}(2)$ .







(d) Rank-3 approximation  $\widehat{A}(3)$ .(e) Rank-4 approximation  $\widehat{A}(4)$ .(f) Rank-5 approximation  $\widehat{A}(5)$ .

# 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 A is its largest singular value  $\sigma_1$ .

# 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:

$$\widehat{A}(k) = \underset{rank(B)=k}{\operatorname{argmin}} \|A - B\|_{2},$$

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

# **Eckart-Young Theorem**

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

### In Summary

Determinants are signed volume of matrices

Matrix decomposition helps in the interpretability of matrices

Matrix approximation is useful in signal compression/approximation

### Pizza



SPECTRAL NORMALIZATION FOR GENERATIVE ADVERSARIAL NETWORKS, Miyato et al ICLR 2018