CS-466/566: Math for AI

Module 05: Singular Value Decomposition

Dr. Mahmoud Mahmoud
The University of Alabama

2026-02-11

TABLE OF CONTENTS

Eigen Decomposition: The “Sum of Patterns” View

General diagonalization: $A = CDC^{-1}$.

For symmetric A: eigenvectors are

orthonormal ($C^{-1} = C^T$), so $A = CDC^T$.

Matrix Multiplication $\rightarrow$ Sum of Rank-1 Matrices:

$$A = \underbrace{\begin{bmatrix} | & & | \\ v_1 & \dots & v_n \\ | & & | \end{bmatrix}}_{V} \underbrace{\begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix}}_{\Lambda} \underbrace{\begin{bmatrix} -v_1^T- \\ \vdots \\ -v_n^T- \end{bmatrix}}_{V^T} = \sum_{i=1}^{n} \underbrace{\lambda_i}_{\text{scalar}} \cdot \underbrace{\mathbf{v}_i}_{n\times 1} \cdot \underbrace{\mathbf{v}_i^T}_{1\times n}$$

Insight: Each term $\lambda_i \mathbf{v}_i \mathbf{v}_i^T$ is an $n \times n$ matrix. If $\lambda_i \approx 0$, that term vanishes $\rightarrow$ **Sparsity / Dimensionality Reduction!**

TABLE OF CONTENTS

Eigen Vectors for Square Matrices Requirement

Let's consider a non-square matrix A:

$$A\mathbf{x} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}_{(3\times2)} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}_{(2\times1)}$$

if $x \in \mathbb{R}^2$ **then** $Ax \in \mathbb{R}^3$

So it can **never** equal $\lambda x \in \mathbb{R}^2$.

Eigen decomposition only works for square matrices!

Why Eigen Decomposition is Not Always Possible

Eigen decomposition / diagonalization assumes:

- A is **square** ($n \times n$)
- and has **enough linearly independent eigenvectors**

But ML data is usually rectangular

- X = (number of samples) $\times$ (number of features)
- e.g., $X \in \mathbb{R}^{10000 \times 768}$

So… How to find a similar concept to eigenvectors for a non-square matrix?

This is exactly why we use SVD.

Trick: Build Two Square Matrices from Any A

Let A be **any** $m \times n$ matrix (maybe not square).

We can always form:

$$AA^T \in \mathbb{R}^{m \times m}, \quad A^T A \in \mathbb{R}^{n \times n}$$

Both are:

- square
- symmetric
- eigenvalues are ≥ 0

So even if A is rectangular, AA^T and $A^T A$ have real eigenvectors.

Why is AA^T Symmetric and Square?

Square: If A is $m \times n$, then A^T is $n \times m$.

$$\underbrace{A}_{m\times n} \cdot \underbrace{A^T}_{n\times m} = \underbrace{AA^T}_{m\times m}$$

$$\underbrace{\begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}}_{3\times 2} \cdot \underbrace{\begin{bmatrix} 1 & 3 & 5 \\ 2 & 4 & 6 \end{bmatrix}}_{2\times 3} = \underbrace{\begin{bmatrix} 5 & 11 & 17 \\ 11 & 25 & 39 \\ 17 & 39 & 61 \end{bmatrix}}_{3\times 3}$$

SVD Roadmap

Our Goal: Factor any $m \times n$ matrix A into $A = U\Sigma V^T$.

The 3-Step Journey:

1. **Find** V?
2. **Find** Σ (Singular values)?
3. **Find** U?

Since A^TA is symmetric → we can always find orthogonal eigenvectors in an indirect way!

SVD Derivation (Part 1)

Step 1: Start with A^TA

We can always find the eigenvalues and eigenvectors of A^TA (even if A is not square):

$$\underbrace{A^TA}_{n\times n}\ \underbrace{\mathbf{v}_i}_{\substack{\text{right eigenvectors}\\ n\times 1}} = \lambda_i\ \underbrace{\mathbf{v}_i}_{\substack{\text{right eigenvectors}\\ n\times 1}}$$

These $\mathbf{v}_i$ are our **Right Singular Vectors**.

Step 2: Define Singular Values

Since $\lambda_i \geq 0$: $\sigma_i = \sqrt{\lambda_i}$

$$\underbrace{A^TA}_{n\times n}\ \underbrace{\mathbf{v}_i}_{\substack{\text{right eigenvectors}\\ n\times 1}} = \sigma_i^2\ \underbrace{\mathbf{v}_i}_{\substack{\text{right eigenvectors}\\ n\times 1}}$$

SVD Derivation (Part 2)

Step 3: Multiply both sides by A:

$$\underbrace{(AA^T)}_{m\times m}\ \underbrace{(A\mathbf{v}_i)}_{\substack{\text{eigenvector!}\\ m\times 1}} = \sigma_i^2\ \underbrace{(A\mathbf{v}_i)}_{\substack{\text{eigenvector!}\\ m\times 1}}$$

So $A\mathbf{v}_i$ is an eigenvector of AA^T!

Define: $\mathbf{u}_i = \frac{A\mathbf{v}_i}{\sigma_i}$ (normalized).

Then: $A\mathbf{v}_i = \sigma_i \mathbf{u}_i \leftarrow$ **core SVD relation!**

Step 4: Stack & Finish

Stack vectors: $\underbrace{V}_{n\times n} = [\mathbf{v}_1, \dots, \mathbf{v}_n], \quad \underbrace{U}_{m\times m} = [\mathbf{u}_1, \dots, \mathbf{u}_m]$

The key relation: $A\mathbf{v}_i = \sigma_i \mathbf{u}_i \implies AV = U\Sigma \implies A = U\Sigma V^T$ ✅

The One Relationship to Remember

SVD gives paired vectors (u_i, v_i) such that:

$$\underbrace{A}_{m\times n} \cdot \underbrace{v_i}_{n\times 1} = \sigma_i \underbrace{u_i}_{m\times 1}$$

Meaning:

- v_i: a special input direction
- Av_i: lands exactly on direction u_i
- scaled by σ_i

So A maps **one special axis** to **another special axis**, with a known scale.

Numeric Example (1/8)

$$A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}_{2\times 3} \quad \Longrightarrow \quad A^T = \begin{bmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{bmatrix}_{3\times 2}$$

Step 1: Compute A^TA:

$$A^TA = \begin{bmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{bmatrix}_{3\times 2} \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}_{2\times 3} = \begin{bmatrix} 13 & 12 & 2 \\ 12 & 13 & -2 \\ 2 & -2 & 8 \end{bmatrix}_{3\times 3}$$

Numeric Example (2/8)

Step 2: Eigenvalues of A^TA — solve $\det(A^TA - \lambda I) = 0$:

$$\det\left(\begin{bmatrix} 13-\lambda & 12 & 2 \\ 12 & 13-\lambda & -2 \\ 2 & -2 & 8-\lambda \end{bmatrix}\right) = 0$$

Cofactor expansion along row 1:

$$= (13-\lambda)\det\begin{bmatrix} 13-\lambda & -2 \\ -2 & 8-\lambda \end{bmatrix} - 12\det\begin{bmatrix} 12 & -2 \\ 2 & 8-\lambda \end{bmatrix} + 2\det\begin{bmatrix} 12 & 13-\lambda \\ 2 & -2 \end{bmatrix}$$

Compute each 2×2 determinant:

$$= (13-\lambda)[(13-\lambda)(8-\lambda) - 4] - 12[12(8-\lambda) + 4] + 2[-24 - 2(13-\lambda)]$$

$$= \lambda^3 - 34\lambda^2 + 225\lambda = \lambda(\lambda-25)(\lambda-9) = 0$$

$$\Longrightarrow \lambda_1 = 25, \quad \lambda_2 = 9, \quad \lambda_3 = 0$$

Numeric Example (3/8)

Step 3: Singular Values ($\sigma = \sqrt{\lambda}$):

$$\sigma_1 = \sqrt{25} = 5, \quad \sigma_2 = \sqrt{9} = 3, \quad \sigma_3 = \sqrt{0} = 0$$

The **non-zero** singular values are $\sigma_1 = 5$ and $\sigma_2 = 3$.

Since A is 2×3, we have at most 2 non-zero singular values.

Numeric Example (4/8): Find V (Part a)

Step 4: Find eigenvectors of A^TA for each λ

For $\lambda_1 = 25$: solve $(A^TA - 25I)\mathbf{v}_1 = 0$

$$\begin{bmatrix} 13-25 & 12 & 2 \\ 12 & 13-25 & -2 \\ 2 & -2 & 8-25 \end{bmatrix}\mathbf{v}_1 = \begin{bmatrix} -12 & 12 & 2 \\ 12 & -12 & -2 \\ 2 & -2 & -17 \end{bmatrix}\mathbf{v}_1 = \mathbf{0}$$

Row reduce → from row 1: $-12v_1 + 12v_2 + 2v_3 = 0 \implies v_1 = v_2 + \frac{v_3}{6}$

Setting $v_3 = 0, v_2 = 1 \implies v_1 = 1$. Normalize:

$$\mathbf{v}_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

Numeric Example (5/8): Find V (Part b)

For $\lambda_2 = 9$: solve $(A^T A - 9I)\mathbf{v}_2 = 0$

$$\begin{bmatrix} 13-9 & 12 & 2 \\ 12 & 13-9 & -2 \\ 2 & -2 & 8-9 \end{bmatrix} \mathbf{v}_2 = \begin{bmatrix} 4 & 12 & 2 \\ 12 & 4 & -2 \\ 2 & -2 & -1 \end{bmatrix} \mathbf{v}_2 = \mathbf{0}$$

Row reduce → solution: $v_1 = 1, v_2 = -1, v_3 = 4$ (proportional). Normalize:

$$\mathbf{v}_2 = \frac{1}{\sqrt{18}} \begin{bmatrix} 1 \\ -1 \\ 4 \end{bmatrix}$$

Numeric Example (6/8): Find V (Part c)

For $\lambda_3 = 0$: solve $(A^T A - 0I)\mathbf{v}_3 = 0$

$$\begin{bmatrix} 13 & 12 & 2 \\ 12 & 13 & -2 \\ 2 & -2 & 8 \end{bmatrix} \mathbf{v}_3 = \mathbf{0}$$

Row reduce → solution: $v_1 = -2, v_2 = 2, v_3 = 1$ (proportional).

Normalize:

$$\mathbf{v}_3 = \frac{1}{3}\begin{bmatrix} -2 \\ 2 \\ 1 \end{bmatrix}$$

Numeric Example (7/8): Find U

Step 5: Find U — use $\mathbf{u}_i = \frac{A\mathbf{v}_i}{\sigma_i}$

$$\mathbf{u}_1 = \frac{1}{\sigma_1} A\mathbf{v}_1 = \frac{1}{5}\begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix} \cdot \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} = \frac{1}{5\sqrt{2}}\begin{bmatrix} 5 \\ 5 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

$$\mathbf{u}_2 = \frac{1}{\sigma_2} A\mathbf{v}_2 = \frac{1}{3}\begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix} \cdot \frac{1}{\sqrt{18}}\begin{bmatrix} 1 \\ -1 \\ 4 \end{bmatrix} = \frac{1}{3\sqrt{18}}\begin{bmatrix} 9 \\ -9 \end{bmatrix} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

Numeric Example (8/8)

Step 6: Build Σ:

$$\Sigma = \begin{bmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix}_{2\times 3}$$

Final Decomposition ($A = U\Sigma V^T$):

$$\underbrace{A}_{2\times 3} = \underbrace{U}_{2\times 2} \cdot \underbrace{\Sigma}_{2\times 3} \cdot \underbrace{V^T}_{3\times 3}$$

$$\Longrightarrow \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix} = \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 5 & 0 & 0 \\ 0 & 3 & 0 \end{bmatrix}}_{\Sigma} \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{18}} & \frac{-1}{\sqrt{18}} & \frac{4}{\sqrt{18}} \\ \frac{-2}{3} & \frac{2}{3} & \frac{1}{3} \end{bmatrix}}_{V^T}$$

TABLE OF CONTENTS

The Best Low-Rank Approximation

SVD allows us to represent an image (matrix A) as a sum of rank-1 patterns:

$$A = \sigma_1 u_1 v_1^T + \sigma_2 u_2 v_2^T + \cdots + \sigma_r u_r v_r^T$$

By keeping only the first k terms, we get the **best possible approximation** of rank k.

Original k=5 k=20 k=50

Original k=5 (Blurry) k=20 (Better) k=50 (Almost Perfect)

TABLE OF CONTENTS

SVD in NumPy

In Python, we use `numpy.linalg.svd`:

```
import numpy as np

#> Compute SVD
U, S, Vt = np.linalg.svd(A, full_matrices=False)
```

Key Details:

1. `S` is returned as a **1D array** (vector), not a diagonal matrix.
2. `Vt` is already transposed (V^T).
3. `full_matrices=False` computes the Economy SVD (faster).

The singular values in S are returned **sorted in descending order**:

$$\sigma_1 \geq \sigma_2 \geq \sigma_3 \geq \cdots \geq 0$$

Reconstructing from SVD

To rebuild the matrix (or an approximation), we need to turn S back into a diagonal matrix:

```
#> Reconstruct A using all components
A_reconst = U @ np.diag(S) @ Vt

#> Approximation with top k components
k = 10
#> S[:k] is the first k elements, np.diag makes it k x k
A_k = U[:, :k] @ np.diag(S[:k]) @ Vt[:k, :]
```

Setting the value of k controls the rank of the approximation:

$$A_k = U \cdot \Sigma_k \cdot V^T$$

TABLE OF CONTENTS

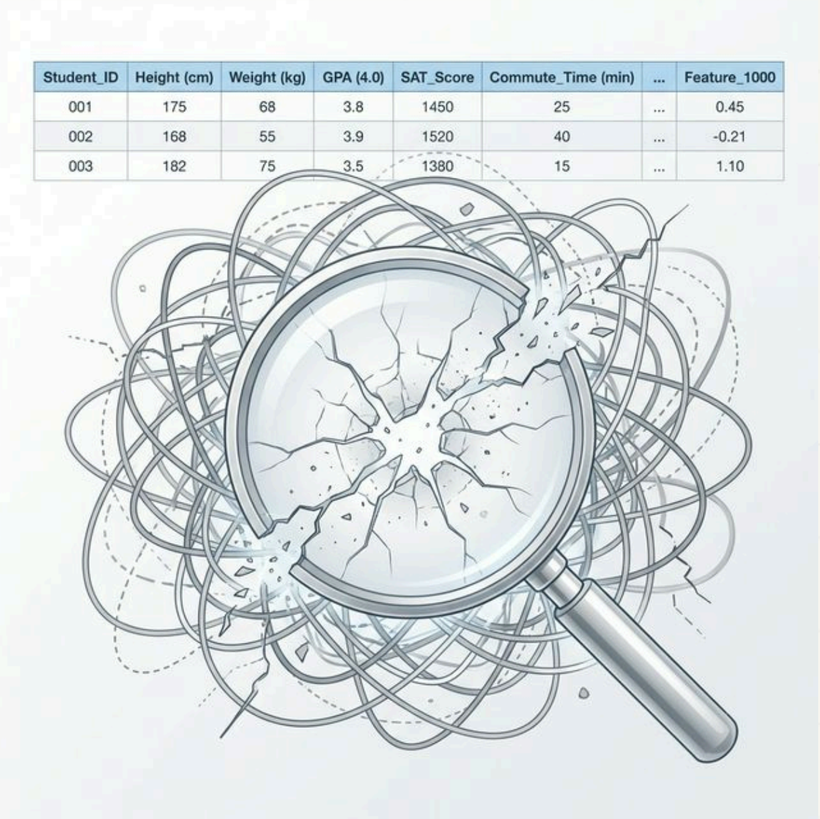
The Curse of Dimensionality

Real-world data has many features:

- Student records: Height, Weight, GPA, SAT, …
- Images: thousands of pixels
- Text: thousands of word frequencies
- Genomics: ~20,000 genes

As dimensions ↑, data becomes **sparse**, distances become **meaningless**, and models **overfit**.

Student_ID	Height (cm)	Weight (kg)	GPA (4.0)	SAT_Score	Commute_Time (min)	...	Feature_1000
001	175	68	3.8	1450	25	...	0.45
002	168	55	3.9	1520	40	...	-0.21
003	182	75	3.5	1380	15	...	1.10

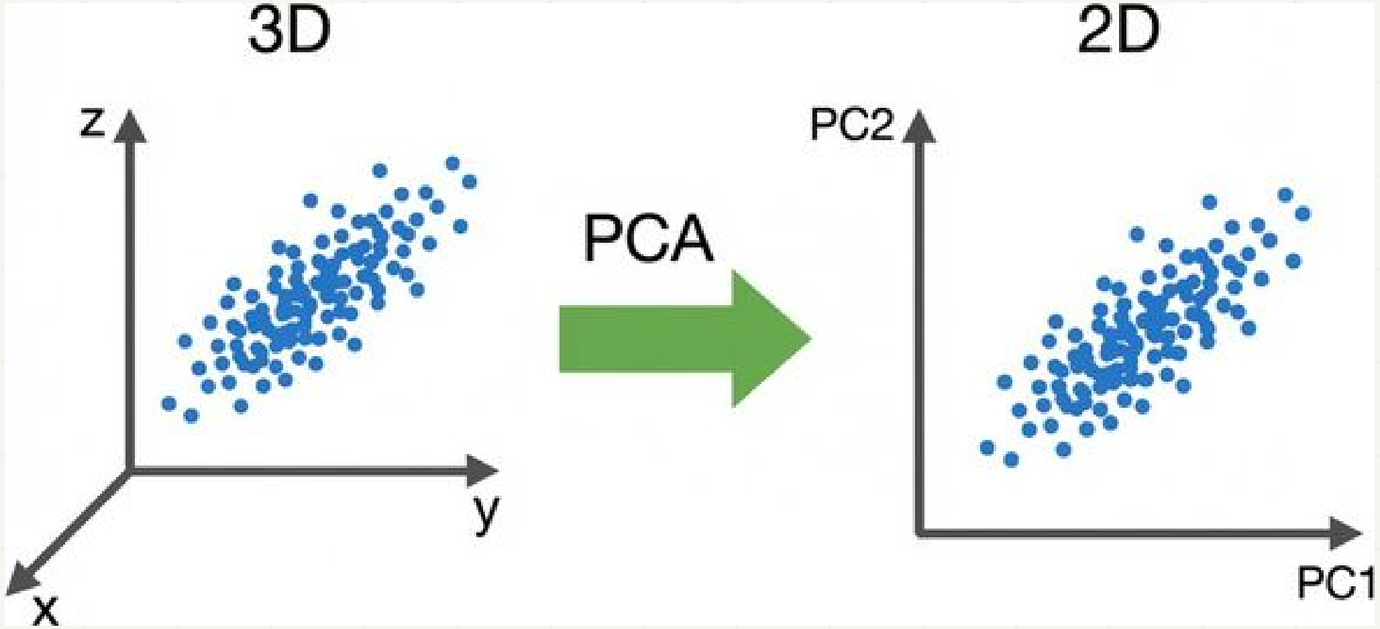


Question: Can we find a *smaller* set of variables that captures most of the information?

What Does PCA Do?

PCA finds a **new coordinate system** where:

1. Axes point along the **directions of maximum variance**
2. Axes are **orthogonal** to each other
3. We can **drop** axes with low variance → dimensionality reduction



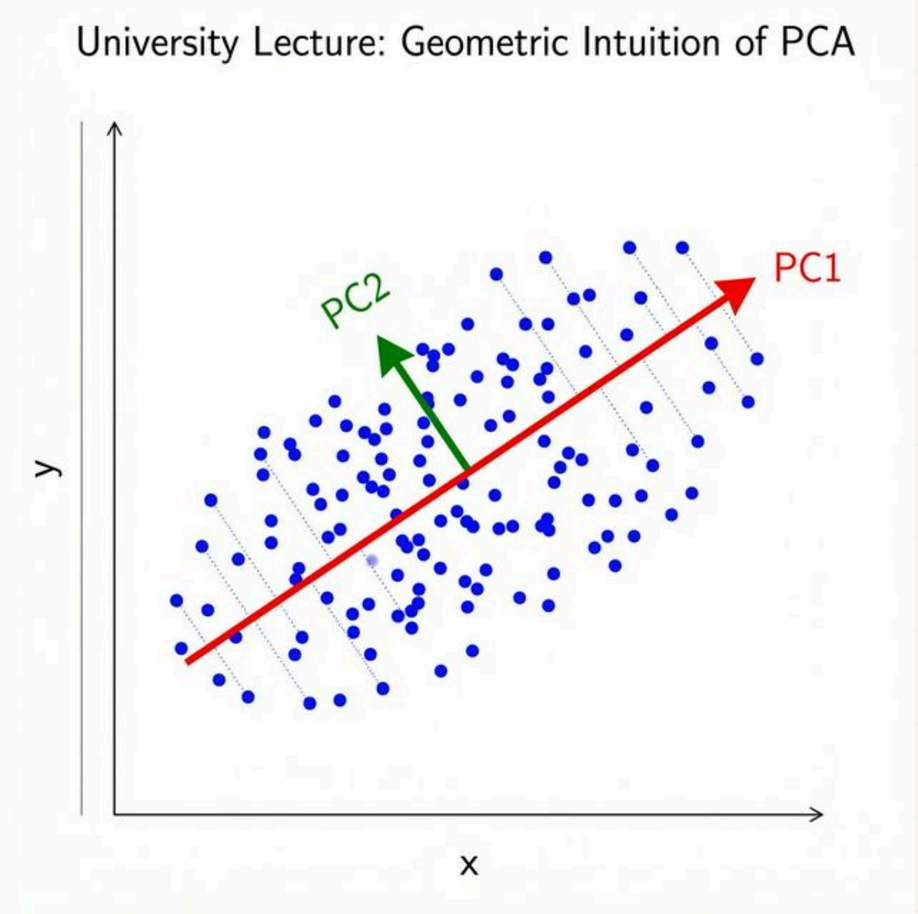
Geometric Intuition

Given a cloud of data points:

- **PC1** = direction of greatest spread (variance)
- **PC2** = direction of greatest spread *perpendicular* to PC1
- **PC3** = … and so on

Each **Principal Component** captures the next most important pattern in the data.

PCA finds the **best linear summary** of your data in fewer dimensions.



PCA Algorithm Summary

Step	Operation	Result
1	Center: $\bar{X} = X - \mathbf{1}\boldsymbol{\mu}^T$	Zero-mean data
2	SVD: $\bar{X} = U\Sigma V^T$	Get components
3	Choose k components	Keep top k columns of V
4	Project: $Z = \bar{X}V_k$	Reduced data ($n \times k$)

Result: We go from d features → k features, where $k \ll d$.

PCA in Python

Using SVD directly (NumPy):

```python
import numpy as np

#> Center the data
X_centered = X - X.mean(axis=0)

#> SVD
U, S, Vt = np.linalg.svd(X_centered, full_matrices=False)

#> Project onto top k components
k = 2
X_reduced = X_centered @ Vt[:k, :].T   # n x k
```

Why Does SVD Give Us the Principal Components?

Step 1: Center the data

Given data matrix X (n samples $\times$ d features), subtract the mean:

$$\bar{X} = X - \mathbf{1}\boldsymbol{\mu}^T$$

Step 2: The covariance matrix is

$$C = \frac{1}{n-1}\bar{X}^T\bar{X}$$

Its eigenvectors = principal components, eigenvalues = variance along each PC.

Step 3: Apply SVD

$\bar{X} = U\Sigma V^T \implies$ the **columns of** V are the principal components!

$$C = \frac{1}{n-1}V\Sigma^2 V^T$$

How Many Components to Keep?

The **variance explained** by each component is:

$$\text{Var explained by PC}_i = \frac{\sigma_i^2}{\sum_{j=1}^{d} \sigma_j^2}$$

Rule of thumb: keep enough components to explain **90-95%** of total variance.

Example: If $\sigma_1 = 10, \sigma_2 = 5, \sigma_3 = 1, \sigma_4 = 0.1$

PC	σ_i^2	% Variance	Cumulative
1	100	79.4%	79.4%
2	25	19.8%	99.2%
3	1	0.8%	100.0%
4	0.01	~0%	100.0%

→ Keeping just **2 PCs** captures **99.2%** of the information!

Thank You!