🔹 Step 1: Start with the Data

We are given two attribute vectors X and Y with **3 samples**:

$$X = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}, \quad Y = \begin{bmatrix} 3 \\ 2 \\ 1 \end{bmatrix}$$

These represent **M = 2 attributes** and **N = 3 samples**.

🔹 Step 2: Center the Data

To center means subtract the **mean** from each value.

🧮 Mean of X:

$$\bar{X} = \frac{1+2+3}{3} = \frac{6}{3} = 2$$

🧮 Mean of Y:

$$\bar{Y} = \frac{3+2+1}{3} = \frac{6}{3} = 2$$

🧮 Centered Vectors:

$$X' = X - \bar{X} = \begin{bmatrix} 1-2 \\ 2-2 \\ 3-2 \end{bmatrix} = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}$$

$$Y' = Y - \bar{Y} = \begin{bmatrix} 3-2 \\ 2-2 \\ 1-2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

🔹 Step 3: Create the Data Matrix

Let’s combine the two centered vectors column-wise:

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

This is our **data matrix** with shape 3×2 (3 rows = samples, 2 columns = attributes).

Step 4: Calculate the Covariance Matrix

Formula for covariance matrix:

$$C = \frac{1}{N} S^T S = \frac{1}{3} S^T S$$

Let's compute S^T first:

$$S^T = \begin{bmatrix} -1 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix}$$

Then:

$$S^T S = \begin{bmatrix} -1 & 0 & 1 \\ 1 & 0 & -1 \end{bmatrix} \cdot \begin{bmatrix} -1 & 1 \\ 0 & 0 \\ 1 & -1 \end{bmatrix} = \begin{bmatrix} (-1)^2 + 0^2 + 1^2 & (-1)(1) + 0(0) + 1(-1) \\ (1)(-1) + 0(0) + (-1)(1) & (1)^2 + 0^2 + (-1)^2 \end{bmatrix}$$

$$= \begin{bmatrix} 1 + 0 + 1 & -1 + 0 - 1 \\ -1 + 0 - 1 & 1 + 0 + 1 \end{bmatrix} = \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix}$$

Now divide by $N = 3$:

$$C = \frac{1}{3} \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix} = \begin{bmatrix} \frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} \end{bmatrix}$$

Step 5: Find Eigenvalues

We solve:

$$\det(C - \lambda I) = 0$$

So,

$$\det\left(\begin{bmatrix} \frac{2}{3} - \lambda & -\frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} - \lambda \end{bmatrix}\right) = 0$$

$$\left(\frac{2}{3} - \lambda\right)^2 - \left(-\frac{2}{3}\right)^2 = 0$$

$$\left(\frac{2}{3} - \lambda\right)^2 - \frac{4}{9} = 0$$

Let $x = \frac{2}{3} - \lambda$, so:

$$x^2 = \frac{4}{9} \Rightarrow x = \pm\frac{2}{3}$$

Then:

- $\frac{2}{3} - \lambda = \frac{2}{3} \Rightarrow \lambda = 0$
- $\frac{2}{3} - \lambda = -\frac{2}{3} \Rightarrow \lambda = \frac{4}{3}$

So:

$$\lambda_1 = 0, \quad \lambda_2 = \frac{4}{3}$$

🔹 Step 6: Find Eigenvectors

For $\lambda_1 = 0$:

Solve:

$$(C - 0I)\mathbf{u} = 0 \Rightarrow C\mathbf{u} = 0$$

$$\begin{bmatrix} \frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

From row 1:

$$\frac{2}{3}u_1 - \frac{2}{3}u_2 = 0 \Rightarrow u_1 = u_2$$

Take:

$$u^{(1)} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \text{normalize it:}$$

$$/\!/ u /\!/ = \sqrt{1^2 + 1^2} = \sqrt{2}, \quad \mathbf{u}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

For $\lambda_2 = \frac{4}{3}$:

Solve:

$$(C - \lambda I)\mathbf{u} = 0 \Rightarrow \left(\begin{bmatrix} \frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} \end{bmatrix} - \frac{4}{3}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\right)\mathbf{u} = 0$$

$$\Rightarrow \begin{bmatrix} -\frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & -\frac{2}{3} \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = 0 \Rightarrow u_1 = -u_2$$

Take:

$$u^{(2)} = \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad // u // = \sqrt{2}, \quad \mathbf{u}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

🔹 Step 7: Create the Eigenvector Matrix U

$$U = \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix} \quad \text{(each column is a normalized eigenvector)}$$

🔹 Step 8: Calculate Principal Components

$$P = S \cdot U$$

Recall:

$$S = \begin{bmatrix} -1 & 1 \\ 0 & 0 \\ 1 & -1 \end{bmatrix}, \quad U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

So,

$$P = \frac{1}{\sqrt{2}} \begin{bmatrix} (-1)(1) + (1)(1) & (-1)(1) + (1)(-1) \\ 0 & 0 \\ (1)(1) + (-1)(1) & (1)(1) + (-1)(-1) \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -2 \\ 0 & 0 \\ 0 & 2 \end{bmatrix}$$

$$P = \begin{bmatrix} 0 & -\sqrt{2} \\ 0 & 0 \\ 0 & \sqrt{2} \end{bmatrix}$$

✅ Final Results Summary

Item	Value
Covariance Matrix	$\begin{bmatrix} \frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} \end{bmatrix}$
Eigenvalues	$\lambda_1 = 0, \lambda_2 = \frac{4}{3}$
Eigenvectors	$u_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, u_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

Item	Value
Principal Component Matrix	$\begin{bmatrix} 0 & -\sqrt{2} \\ 0 & 0 \\ 0 & \sqrt{2} \end{bmatrix}$

✅ FINAL CONCLUSION: What Happened in Our PCA Analysis

🎯 Goal of PCA

The purpose of **Principal Component Analysis (PCA)** is to:

1. Reduce **dimensionality** of data.
2. Find **new axes** (principal components) that:
   - Capture the **maximum variance** in the data.
   - Are **orthogonal** (uncorrelated).
   - Help interpret the underlying structure.

In our case, we had a **2D dataset (X and Y)** with **3 samples**.

📊 Step-by-Step Outcome

✅ 1. We Centered the Data

We removed the mean from both X and Y so that the data is centered around the origin.
This is crucial because PCA depends on variance from the origin.

Result:

$$X' = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \quad Y' = \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}$$

✅ 2. We Computed the Covariance Matrix

The covariance matrix captures how X and Y vary **with respect to each other**.

We calculated:

$$C = \frac{1}{3} \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix} = \begin{bmatrix} \frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} \end{bmatrix}$$

This tells us:

- Variance of X and Y: $\frac{2}{3}$
- Strong **negative correlation** between X and Y (cross terms = −⅔)

✅ 3. We Found Eigenvalues and Eigenvectors

We solved for:

- **Eigenvalues** $\lambda_1 = 0, \lambda_2 = \frac{4}{3}$
- **Eigenvectors** (directions of principal components):
  - $\mathbf{u}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}$
  - $\mathbf{u}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

Interpretation:

- The **first principal component direction** u_2 (with eigenvalue $\frac{4}{3}$) captures **all the variance**.
- The second component u_1 (with eigenvalue 0) captures **no variance** — it's **redundant**.

✅ 4. We Projected the Data to New Axes (PCA Transform)

Using matrix multiplication $P = S \cdot U$, we projected the data onto the new axes (principal components).

We obtained:

$$P = \begin{bmatrix} 0 & -\sqrt{2} \\ 0 & 0 \\ 0 & \sqrt{2} \end{bmatrix}$$

This is the transformed data in the new space.

🧠 What Does the Final Outcome Tell Us?

📌 1. Only One Meaningful Direction Exists

- All the variation in the original data lies **along one direction**, specifically:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

- The **second direction (perpendicular to this)** has **no spread** — all projected values are 0.

📌 2. Dimensionality Reduction Is Possible

- We started with **2D data**.
- PCA shows that we can represent the **entire dataset in 1D** without losing any variance.
- This is **compression without loss**.

📌 3. Decorrelation Achieved

- Original X and Y were **negatively correlated**.
- PCA transforms the data into **uncorrelated axes** (principal components).

🔚 Conclusion Summary

- We successfully applied PCA to a simple 2D dataset.
- We centered the data, computed the covariance matrix, and solved for eigenvalues/eigenvectors.

- The PCA transformation rotated the data such that all the variance is along **one principal axis.**
- This transformation allowed us to **reduce the dimensionality from 2D to 1D** while retaining **100% of the information.**

This example **demonstrates the core idea of PCA**: rotate the data to align with its most informative directions and simplify it without losing key information.

> ✅ PCA allows us to represent the **entire dataset** in **1D** (along one principal component) **without losing any variance**.

We'll demonstrate this in **three exact steps**:

🔁 Recap of the Key Values

We had:

Centered data matrix S:

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

Covariance matrix C (with division by $N = 3$):

$$C = \frac{1}{3} S^T S = [\begin{matrix} \frac{2}{3} & -\frac{2}{3} \\ -\frac{2}{3} & \frac{2}{3} \end{matrix}]$$

Eigenvalues:

- $\lambda_1 = 0$

- $\lambda_2 = \frac{1}{3}$

So **total variance** in original data = sum of eigenvalues:

$$\text{Total Variance} = \lambda_1 + \lambda_2 = 0 + \frac{4}{3} = \frac{4}{3}$$

✅ Step 1: Show Variance Captured by Each Principal Component

We now project the data onto each principal component and compute **variance of each**.

Principal components matrix $P = S \cdot U$:

Where $U = [\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix}, \frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}]$

We got:

$$P = \begin{bmatrix} 0 & -\sqrt{2} \\ 0 & 0 \\ 0 & \sqrt{2} \end{bmatrix}$$

Let's extract each component:

- **First Principal Component** (PC1) — column 1 of P:

$$PC_1 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad \Rightarrow \text{Variance} = 0$$

- **Second Principal Component** (PC2) — column 2 of P:

$$PC_2 = \begin{bmatrix} -\sqrt{2} \\ 0 \\ \sqrt{2} \end{bmatrix}$$

Now compute variance of PC2:

$$\text{Mean of PC2} = \frac{-\sqrt{2} + 0 + \sqrt{2}}{3} = 0$$

$$\text{Variance} = \frac{1}{3}[(-\sqrt{2})^2 + 0^2 + (\sqrt{2})^2] = \frac{1}{3}(2 + 0 + 2) = \frac{4}{3}$$

✅ Step 2: Verify Total Variance Is Preserved

- **Variance in original data:** $\frac{4}{3}$
- **Variance in PC2 (the only informative component):** $\frac{4}{3}$
- **Variance in PC1 (discarded component):** 0

✅ **All the variance is captured in PC2.**

✅ Step 3: Explain Why This Means Dimensionality Reduction Without Loss

- The original data was 2-dimensional (X and Y).
- PCA transformed it to new axes: PC1 and PC2.
- Only **PC2 has non-zero variance**, i.e., **all spread, all information is along PC2**.
- PC1 = 0 ⇒ no useful information exists in that direction.

Thus, we can **safely discard PC1** and retain only PC2:

$$\text{New 1D representation} = PC_2 = \begin{bmatrix} -\sqrt{2} \\ 0 \\ \sqrt{2} \end{bmatrix}$$

From this **1D vector**, we can **reconstruct the original centered data** using:

$$\tilde{S} = PC_2 \cdot (u_2)^T = \begin{bmatrix} -\sqrt{2} \\ 0 \\ \sqrt{2} \end{bmatrix} \cdot \left(\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 \end{bmatrix}\right) \Rightarrow \begin{bmatrix} -1 & 1 \\ 0 & 0 \\ 1 & -1 \end{bmatrix}$$

✅ Exactly matches original centered matrix S!

🔚 Conclusion (Proven)

- **All original variance** is preserved in **just 1 principal component** (PC2).
- The **first component** has **0 variance** and can be discarded.
- We successfully **reduced dimensions from 2D to 1D.**
- The **entire dataset** can be perfectly represented in this **single direction**, with **no loss of information**.