Understanding Principal Component Analysis (PCA) with a Numerical Example

Introduction

Principal Component Analysis (PCA) is a powerful dimensionality reduction technique commonly used in machine learning and data analysis. The main objective of PCA is to reduce the number of features (dimensions) in a dataset while preserving as much variance as possible. This makes it easier to visualize and interpret the data, especially in the case of high-dimensional datasets.

In this article, we'll walk through PCA step-by-step using a simple 2D dataset.

Dataset

Let's consider a small dataset with two features, **Feature 1** (x) and **Feature 2** (x). The data is as follows:

Observation	Feature 1 (x)	Feature 2 (x)
1	2	3
2	3	4
3	4	5
4	5	6
5	6	7

This is a simple 2D dataset where each row represents a different observation and the two columns represent two features.

Step 1: Standardize the Data

Before applying PCA, it's crucial to standardize the data. Standardization transforms the features so that each feature has a mean of 0 and a variance of 1. This ensures that no feature dominates due to its scale.

1.1 Calculate the Mean of Each Feature First, calculate the mean for each feature:

$$\mu_1 = \frac{2+3+4+5+6}{5} = 4$$
$$\mu_2 = \frac{3+4+5+6+7}{5} = 5$$

1.2 Center the Data Next, subtract the mean from each feature value. This will center the data around zero:

For Feature 1 (x):

$$2-4=-2, \quad 3-4=-1, \quad 4-4=0, \quad 5-4=1, \quad 6-4=2$$

For Feature 2 (x):

$$3-5=-2, \quad 4-5=-1, \quad 5-5=0, \quad 6-5=1, \quad 7-5=2$$

Thus, the **centered data** becomes:

Observation	Centered Feature 1 (x)	Centered Feature 2 (x)
1	-2	-2
2	-1	-1
3	0	0
4	1	1
5	2	2

Normalizing vs. Standardizing Data

Before applying PCA, data often needs to be preprocessed, either through **normalization** or **standardization**. The image below shows the effects of normalization and standardization:

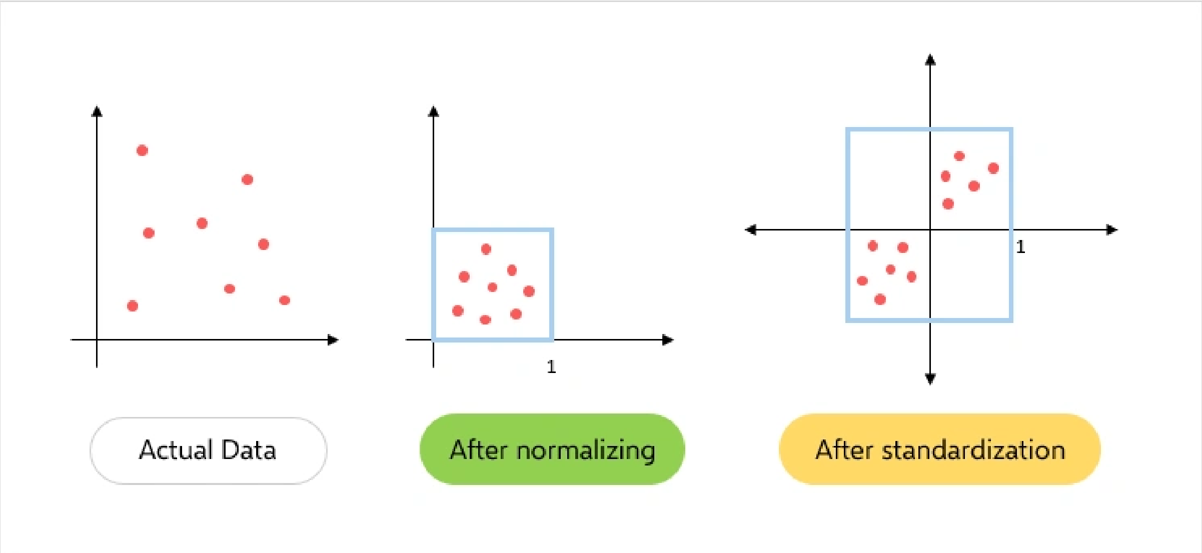

Figure 1: (Image credit: `https://www.analyticsvidhya.com`)

Step 2: Calculate the Covariance Matrix

The covariance matrix tells us how the features vary together. It is a key component of PCA, as it captures the relationships between the features.

$$\mathrm{Cov}(X) = \begin{bmatrix} \mathrm{Var}(x_1) & \mathrm{Cov}(x_1, x_2) \\ \mathrm{Cov}(x_1, x_2) & \mathrm{Var}(x_2) \end{bmatrix}$$

2.1 Calculate the Variance and Covariance
The formulas for variance and covariance are as follows:

$$\mathrm{Var}(x) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \mu_x)^2$$

$$\mathrm{Cov}(x, y) = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \mu_x)(y_i - \mu_y)$$

Variance of Feature 1 (x):

$$\mathrm{Var}(x) = \frac{(-2)^2 + (-1)^2 + (0)^2 + (1)^2 + (2)^2}{5-1} = \frac{4+1+0+1+4}{4} = 2.5$$

Variance of Feature 2 (x):

$$\mathrm{Var}(x) = \frac{(-2)^2 + (-1)^2 + (0)^2 + (1)^2 + (2)^2}{5-1} = \frac{4+1+0+1+4}{4} = 2.5$$

Covariance between Feature 1 and Feature 2:

$$\text{Cov}(x, x) = \frac{(-2)(-2) + (-1)(-1) + (0)(0) + (1)(1) + (2)(2)}{5 - 1} = \frac{4 + 1 + 0 + 1 + 4}{4} = 2.5$$

Thus, the covariance matrix is:

$$\text{Cov}(X) = \begin{bmatrix} 2.5 & 2.5 \\ 2.5 & 2.5 \end{bmatrix}$$

Step 3: Compute Eigenvalues and Eigenvectors

PCA relies on the eigenvectors and eigenvalues of the covariance matrix. These eigenvectors represent the principal components of the data, and the eigenvalues represent the amount of variance captured by each principal component.

We solve for the eigenvalues and eigenvectors of the covariance matrix using the determinant equation:

$$\det(\text{Cov}(X) - \lambda I) = 0$$

Where λ represents the eigenvalues, and I is the identity matrix.
Eigenvalues:
I have directly written the values , you can calucalate this by yourself.
The eigenvalues of the covariance matrix are:

$$\lambda_1 = 5, \quad \lambda_2 = 0$$

Eigenvectors: The eigenvectors corresponding to these eigenvalues are:

$$\mathbf{v}_1 = \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}, \quad \mathbf{v}_2 = \begin{bmatrix} -0.707 \\ 0.707 \end{bmatrix}$$

Step 4: Sort Eigenvalues and Select Principal Components

We sort the eigenvalues in descending order and select the eigenvector corresponding to the highest eigenvalue. In this case, the eigenvalue $\lambda_1 = 5$ is larger, so we select the eigenvector corresponding to λ_1:

$$\mathbf{v}_1 = \begin{bmatrix} 0.707 \\ 0.707 \end{bmatrix}$$

This eigenvector represents the direction of the first principal component.

Step 5: Project the Data onto the First Principal Component

Finally, we reduce the dimensionality of the dataset by projecting the data onto the first principal component. The projected data is obtained by multiplying the centered data by the eigenvector:

$$\text{Projected Data} = X \cdot \mathbf{v}_1$$

For each observation, the projection onto the first principal component is calculated:

$$\text{Observation 1:} \quad (-2 \cdot 0.707) + (-2 \cdot 0.707) = -2.828$$

$$\text{Observation 2:} \quad (-1 \cdot 0.707) + (-1 \cdot 0.707) = -1.414$$

$$\text{Observation 3:} \quad (0 \cdot 0.707) + (0 \cdot 0.707) = 0$$

$$\text{Observation 4:} \quad (1 \cdot 0.707) + (1 \cdot 0.707) = 1.414$$

$$\text{Observation 5:} \quad (2 \cdot 0.707) + (2 \cdot 0.707) = 2.828$$

Thus, the transformed (reduced) data is:

Observation	First Principal Component
1	-2.828
2	-1.414
3	0
4	1.414
5	2.828

This represents the data in a 1-dimensional space, capturing the maximum variance in the original 2D dataset.

Conclusion

Principal Component Analysis (PCA) is a commonly utilized unsupervised learning technique for reducing the dimensionality of data. We trust this article has clarified the concept of PCA and highlighted its practical uses.