Principle Component Analysis – Computation Demo

(This material has been generated from Gen AI tools. This is for demonstration purpose.)

Let's work through a step-by-step example of Principal Component Analysis (PCA) for a small, 2-dimensional dataset. We'll track the data transformation through the key mathematical phases.

Example Dataset and Goal

Suppose we have five data points, X, with two features, x_1 and x_2:

Point ID	x1	x2
1	2.5	2.5
2	0.5	4.5
3	2.2	2.9
4	1.9	2.2
5	3.1	3.0

Goal: Reduce the dimensionality from 2D to 1D using the principal component that captures the most variance.

Step 1: Standardize the Data (Centering)

PCA is sensitive to the scale of features, so we first **center** the data by subtracting the mean of each feature from all its values.

A. Calculate Means

$$\bar{x}_1 = \frac{2.5 + 0.5 + 2.2 + 1.9 + 3.1}{5} = 2.04$$

$$\bar{x}_2 = \frac{2.5 + 4.5 + 2.9 + 2.2 + 3.0}{5} = 3.02$$

B. Center the Data (X_centered)

$$x_i' = x_i - \bar{x}$$

Point ID	x1'	x2'
1	0.46	-0.52
2	-1.54	1.48
3	0.16	-0.12
4	-0.14	-0.82
5	1.06	-0.02

Step 2: Calculate the Covariance Matrix (Σ)

The covariance matrix measures the variance of each feature and the covariance (relationship) between feature pairs. Since the data is centered, we use:

$$\Sigma = \frac{1}{n-1}\mathbf{X}_{centered}^T \mathbf{X}_{centered}$$

The covariance matrix for this data is calculated as:

$$\Sigma \approx \begin{pmatrix} \mathrm{Var}(x_1') & \mathrm{Cov}(x_1', x_2') \\ \mathrm{Cov}(x_2', x_1') & \mathrm{Var}(x_2') \end{pmatrix} = \begin{pmatrix} 0.73 & -0.22 \\ -0.22 & 0.88 \end{pmatrix}$$

Note 1: **Var(x_1') is 0.73**, **Var(x_2') is 0.88**, and **Cov(x_1', x_2') is -0.22**. The negative covariance suggests the features are slightly inversely related.

Note 2: When computed, I got Var(x_1') = 0.94, Var(x_2') = 0.79 and Cov(x_1', x_2') = 0.61. Despite the differences, the process of calculation is the same.

Step 3: Find Eigenvalues and Eigenvectors

The eigenvectors of the covariance matrix are the **Principal Components (PCs)**, and the eigenvalues represent the **variance** captured along those PCs.

We solve the characteristic equation $\det(\Sigma - \lambda\mathbf{I}) = 0.$

A. Eigenvalues (λ)

Solving the quadratic equation results in two eigenvalues:

$$\lambda_1 \approx \mathbf{0.99}$$

$$\lambda_2 \approx \mathbf{0.62}$$

B. Eigenvectors (v)

For each eigenvalue, we solve the equation $(\Sigma - \lambda\mathbf{I})\mathbf{v} = \mathbf{0}$ to find the corresponding eigenvector.

- **PC1 (for $\lambda_1 = 0.99$): $\mathbf{v}_1 \approx \begin{pmatrix} -0.47 \\ 0.88 \end{pmatrix}$**
  - This component captures 0.99 units of variance.
- **PC2 (for $\lambda_2 = 0.62$): $\mathbf{v}_2 \approx \begin{pmatrix} 0.88 \\ 0.47 \end{pmatrix}$**
  - This component captures 0.62 units of variance.

Step 4: Select Principal Components

We rank the PCs by their eigenvalues (λ). Since $\lambda_1 > \lambda_2$, **PC1** is the most important component.

A. Explained Variance Ratio

The total variance is λ_1 + λ_2 = 0.99 + 0.62 = 1.61.

- **PC1 Ratio:** $\frac{0.99}{1.61} \approx \mathbf{61.5\%}$
- **PC2 Ratio:** $\frac{0.62}{1.61} \approx \mathbf{38.5\%}$

Since PC1 captures the majority (61.5%) of the variance, we choose to keep only **PC1** to reduce the dimensionality to 1D.

Step 5: Transform the Data

We project the centered data ($\mathbf{X}_{centered}$) onto the selected eigenvector ($\mathbf{v}_1$) to get the final reduced dataset ($\mathbf{Z}$).

$$\mathbf{Z} = \mathbf{X}_{centered} \cdot \mathbf{v}_1$$

$$\mathbf{Z} = \begin{pmatrix} 0.46 & -0.52 \\ -1.54 & 1.48 \\ 0.16 & -0.12 \\ -0.14 & -0.82 \\ 1.06 & -0.02 \end{pmatrix} \cdot \begin{pmatrix} -0.47 \\ 0.88 \end{pmatrix}$$

Final 1D Scores

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We calculate the dot product for each row:

- $Z_1 = (0.46 \cdot -0.47) + (-0.52 \cdot 0.88) \approx -0.216 - 0.458 = -\mathbf{0.674}$
- $Z_2 = (-1.54 \cdot -0.47) + (1.48 \cdot 0.88) \approx 0.724 + 1.302 = \mathbf{2.026}$
- $Z_3 = (0.16 \cdot -0.47) + (-0.12 \cdot 0.88) \approx -0.075 - 0.106 = -\mathbf{0.181}$
- $Z_4 = (-0.14 \cdot -0.47) + (-0.82 \cdot 0.88) \approx 0.066 - 0.722 = -\mathbf{0.656}$
- $Z_5 = (1.06 \cdot -0.47) + (-0.02 \cdot 0.88) \approx -0.498 - 0.017 = -\mathbf{0.515}$

The original 5x2 dataset is now reduced to a 5x1 dataset: $\mathbf{Z} = \begin{pmatrix} -0.674 \\ 2.026 \\ -0.181 \\ -0.656 \\ -0.515 \end{pmatrix}$. This single column preserves 61.5% of the original data's total variance.

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