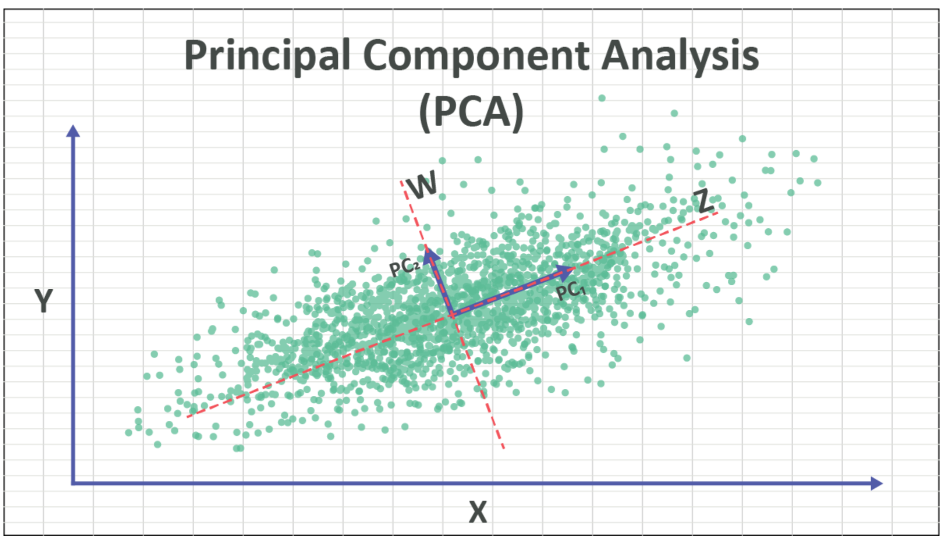
Principal Component Analysis

Introduction

Principal Component Analysis (PCA) is an unsupervised dimensionality reduction technique used to reduce the number of features in a dataset while preserving as much variance as possible. PCA is widely used for data visualization, noise reduction, and preprocessing prior to supervised learning. PCA identifies new, uncorrelated variables (called principal components) that capture the most significant patterns in the data.



Core Concepts

- Principal Components: New axes (linear combinations of the original features) along which the data variance is maximized.
- Orthogonality: Principal components are orthogonal to each other.
- Variance Maximization: PCA seeks the directions of maximum variance in the data.

Mathematical Formulation

Given a centered dataset $X \in \mathbb{R}^{n \times d}$ with n samples and d features:

1. Compute the covariance matrix:
$$\Sigma = \frac{1}{n} X^T X \tag{1}$$
2. Perform eigendecomposition on Σ:
$$\Sigma v_i = \lambda_i v_i \tag{2}$$
where v_i are eigenvectors (principal directions) and λ_i are eigenvalues (explained variance).
3. Select the top k eigenvectors corresponding to the k largest eigenvalues.
4. Project the data onto the new k-dimensional subspace:
$$Z = XW_k \tag{3}$$
where W_k contains the top k eigenvectors as columns.

Explained Variance Ratio

The proportion of total variance explained by the j-th principal component is:

$$\text{Explained Variance Ratio}_j = \frac{\lambda_j}{\sum_{i=1}^{d} \lambda_i} \tag{4}$$

Key Characteristics

- Type: Unsupervised linear dimensionality reduction.
- Goal: Maximize variance captured in fewer dimensions.
- Data Requirement: Data must be centered (zero means).
- Output: Uncorrelated components ordered by explained variance.

Strengths

- Reduces computational cost and risk of overfitting.
- Helps visualize high-dimensional data.
- Removes multicollinearity by creating uncorrelated features.
- Retains the most important variation in the data.

Weaknesses

- Components are hard to interpret.
- Assumes linear relationships.
- Sensitive to feature scaling.
- Does not preserve class separability.

Applications of PCA

- Data Visualization: Reducing to 2D or 3D for plotting.
- Preprocessing: Noise reduction and decorrelation before classification.
- Compression: Storing reduced feature representations.
- Gene Expression Analysis: Extracting patterns in biological data.

Conclusion

Principal Component Analysis is a fundamental tool in unsupervised learning, offering a principled approach to simplify complex datasets. While it comes with interpretability trade-offs, PCA remains highly effective for dimensionality reduction and exploratory analysis.