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Principal Component Analysis (PCA)

- It is a Feature Extraction algorithm, not a feature selection, convert n features to k , where $k < n$
- **Principal Component Analysis (PCA)** is one of the most popular techniques for dimensionality reduction
- PCA transforms the original features into a new set of uncorrelated features called **principal components**
- These components are ordered by the amount of variance they capture from the data, with the first few components capturing most of the variability

Working of PCA

1. Standardize the Data

- Ensure that the data is centered around the origin (mean = 0) and has unit variance

$$X_{\text{std}} = \frac{X - \mu}{\sigma}$$

- where μ is the mean of the data, and σ is the standard deviation

2. Compute the Covariance Matrix

- The covariance matrix is a square matrix that shows the covariance (a measure of how much two variables change together) between pairs of features in the data

$$\mathbf{C} = \frac{1}{n-1} \mathbf{X}_{\text{std}}^T \mathbf{X}_{\text{std}}$$

$$\mathbf{C} = \frac{1}{n-1} \sum_{i=1}^n (\mathbf{x}_i - \mu)(\mathbf{x}_i - \mu)^T$$

3. Compute the Eigenvalues and Eigenvectors

- **Eigenvalues** : Indicate the amount of variance captured by each eigenvector (principal component)
- **Eigenvectors** : Represent the directions of the principal components in the feature space

$$\mathbf{C}\mathbf{v} = \lambda\mathbf{v}$$

- where (λ) is the eigenvalue and (\mathbf{v}) is the corresponding eigenvector

4. Sort Eigenvectors by Eigenvalues

- The eigenvectors are sorted in decreasing order of their corresponding eigenvalues

- The top eigenvectors (with the largest eigenvalues) are chosen to form the new feature space

5. Transform the Data

- The original data is projected onto the selected eigenvectors (principal components), creating a new dataset with reduced dimensions

$$\mathbf{X}_{\text{pca}} = \mathbf{X}_{\text{std}} \mathbf{V}$$

- where (\mathbf{V}) is the matrix of the top (k) eigenvectors

6. Variance Explained by Each Principal Component

$$\text{Variance}(\text{Component } i) = \frac{\lambda_i}{\sum_{j=1}^k \lambda_j}$$

Objective of PCA

- **Maximizing Variance**
- **Minimizing Distances**

Intuition Behind PCA

- PCA seeks to find new axes (principal components) that maximize the variance in the data
- The first principal component captures the most variance, and each subsequent component captures the maximum remaining variance while being orthogonal to the previous components

Advantages of PCA

- **Reduces Complexity** : By focusing on the most significant components, PCA simplifies the dataset
- **De-correlates Features** : The resulting principal components are uncorrelated, which can improve the performance of machine learning algorithms
- **Facilitates Visualization** : PCA can reduce data to 2D or 3D for easy visualization

Limitations of PCA

- **Loss of Information** : Some data variance is inevitably lost when reducing dimensions
- **Assumption of Linearity** : PCA assumes that the principal components are linear combinations of the original features, which may not capture complex, nonlinear relationships
- **Interpretability** : The new components may not have a clear or interpretable meaning

Applications of PCA

- **Data/Image Compression** : Reducing the dimensionality of image data while preserving key features
- **Noise Reduction** : Eliminating noise by discarding low-variance components
- **Feature Extraction** : Selecting the most important features from a large set for better model performance
- **Data Visualization** : reducing the dimension to 2D or 3D, in order to visualize the dataset
- **Speed Up Computation** : reduces load on memory