Principal Component Analysis

2017

Overview

1. Eigenvectors and Eigenvalues
2. Principal Component Analysis
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Eigenvectors and Eigenvalues

A vector $v \in \mathbb{R}^n$ is an *eigenvector* of a matrix $A \in \mathbb{R}^{n \times n}$ if

$$Av = \lambda v \tag{1}$$

where λ is a scalar called the *eigenvalue* associated with v. Eigenvectors (values) are found by solving (1)

$$(A - \lambda I)v = 0 \tag{2}$$

Eq. (2) has a non-zero solution v only if

$$\det(A - \lambda I) = 0 \tag{3}$$

Eigenvectors and Eigenvalues

Example: find the eigenvectors and eigenvalues of matrix

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 3 \end{bmatrix}$$

Solving (3), we get

$$\begin{aligned} & A - \lambda I = \begin{bmatrix} 1 - \lambda & 0 \\ 1 & 3 - \lambda \end{bmatrix} \\ & \Rightarrow \det(A - \lambda I) = (1 - \lambda)(3 - \lambda) \\ & \Rightarrow \lambda_1 = 1, \lambda_2 = 3 \end{aligned}$$

Two eigenvalues $\lambda_1, \lambda_2 \Rightarrow$ two eigenvectors v_1, v_2.

Eigenvectors and Eigenvalues

Plugging λ_1 and λ_2 into (1) we have

$$\begin{bmatrix} 1 & 0 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix} = 1 \begin{bmatrix} v_{11} \\ v_{12} \end{bmatrix}$$
$$\begin{bmatrix} 1 & 0 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} v_{21} \\ v_{22} \end{bmatrix} = 3 \begin{bmatrix} v_{21} \\ v_{22} \end{bmatrix}$$

From which we get $v_{11} = -2v_{12}$, $v_{21} = 0$ and $v_{22} \in \mathbb{R}$. That is:

- any vector $v_1 = [v_{11} \; v_{12}]^T$ where $v_{11} = -2v_{22}$ is an eigenvector of A with eigenvalue $\lambda_1 = 1$.
- any vector $v_2 = [v_{21} \; v_{22}]^T$ where $v_{21} = 0$ and $v_{22} \in \mathbb{R}$ is an eigenvector of A with eigenvalue $\lambda_2 = 3$.

Eigendecomposition

Decomposing a square matrix into its eigenvectors and eigenvalues is called *eigendecomposition*.

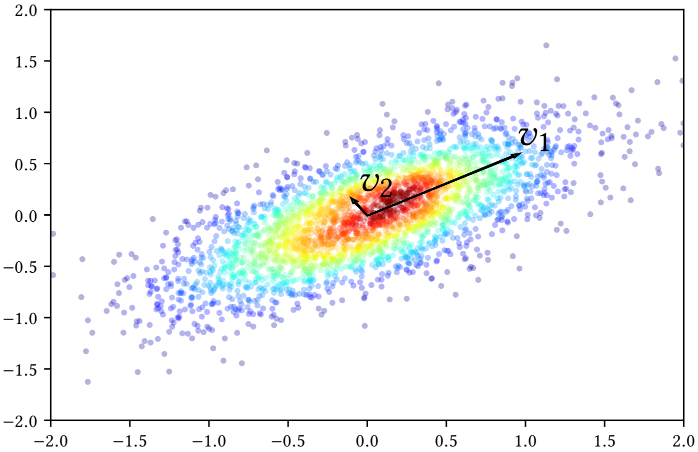
- *eigenvectors* are vectors which are fixed in direction under a given linear transformation
- the scaling factor of these eigenvectors is then called the *eigenvalue*

Suppose we have a set of data with a certain distribution.

- eigenvectors v_i tell us the orientation of the distribution
- eigenvalues λ_i tell the variance in each dimension

Eigendecomposition

$$\Sigma = \begin{bmatrix} 0.3 & 0.2 \\ 0.2 & 0.3 \end{bmatrix},\ v = \begin{bmatrix} 0.707 & -0.707 \\ 0.707 & 0.707 \end{bmatrix},\ \lambda = \begin{bmatrix} 0.5 \\ 0.1 \end{bmatrix}$$



Principal Component Analysis

- Reduce the dimensionality of the original feature set by projecting onto a smaller subspace, where the *eigenvectors* will form the axes.
- We use the corresponding *eigenvalues* to choose which dimensions to include. The new dimensions are *principal components*.

Principal Component Analysis

Example: Iris Dataset

- R. A. Fisher, *The Use of Multiple Measurements in Taxonomic Problems*, 1936
- Data describing the morphologic variation of Iris flowers of three related species (three class labels)
- Four features: the length and width of the sepals and petals, in centimeters

(a) Iris-setosa

(b) Iris-versicolor

(c) Iris-virginica

(source: https://en.wikipedia.org/wiki/Iris_flower_data_set)

Principal Component Analysis

Example: Iris Dataset

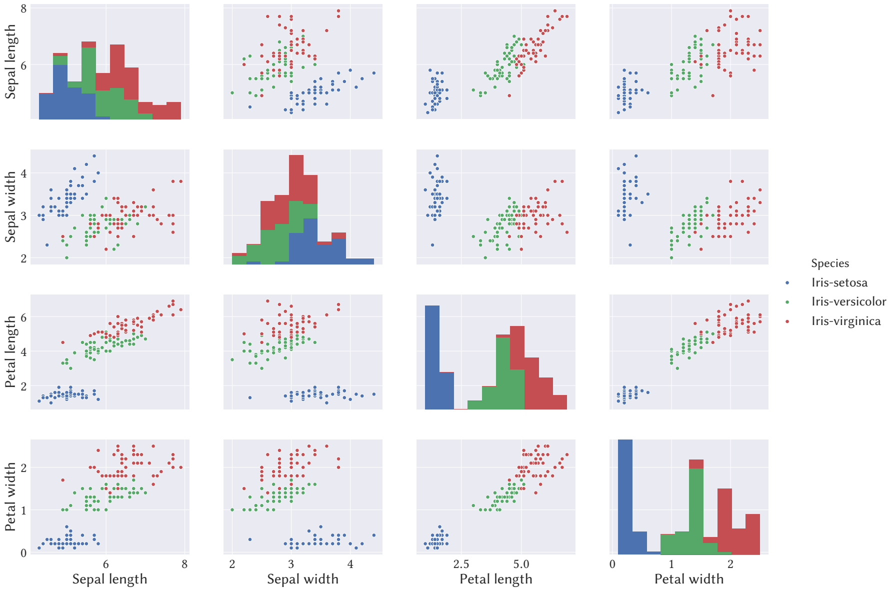
Input data $\mathbf{X}$

$$\mathbf{x}^T = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} \text{Sepal length} \\ \text{Sepal width} \\ \text{Petal length} \\ \text{Petal width} \end{bmatrix}$$

- 150 instances (50 for each class), no missing values
- Predicted attribute: species

Principal Component Analysis

Example: Iris Dataset



Principal Component Analysis

Example: Iris Dataset

Step-by-step guide

1. Standardize the data (mean = 0, variance = 1)
2. Calculate *eigenvectors* and *eigenvalues*
3. Choose k principal components based on the k largest *eigenvalues*
4. Construct projection matrix $\mathbf{W}$ from the selected k *eigenvectors*
5. Transform original feature space $\mathbf{X}$ using $\mathbf{W}$ to obtain k-dimensional feature subspace $\mathbf{Y}$

$$\overbrace{\mathbf{Y}}^{\text{Projected data}} = \underbrace{\mathbf{X}}_{\text{Original data}} \cdot \overbrace{\mathbf{W}}^{\text{Projection matrix}}$$

Principal Component Analysis

Example: Iris Dataset

1. Standardization (Z-score normalization)
   - Transform the data to have zero mean and unit variance

$$x' = \frac{x - \mu}{\sigma}$$

   - Important step for many machine learning algorithms (eg., k-means, k-NN, SVM, LDA, PCA, logistic regression)
   - When in doubt, standardize

Principal Component Analysis

Example: Iris Dataset

2. Eigenvectors and eigenvalues
   - Eigendecomposition of covariance matrix Σ, where

$$\sigma_{jk} = \frac{1}{n-1} \sum_{i=1}^{n} (x_{ij} - \overline{x}_j)(x_{ik} - \overline{x}_k)$$

   - We can also use the correlation matrix $\mathrm{corr}(\mathbf{X})$ where

$$r_{jk} = \frac{\sum_{i=1}^{n} (x_{ij} - \overline{x}_j)(x_{ik} - \overline{x}_k)}{(n-1) s_j s_k}$$

   - In practice, we prefer singular value decomposition (computationally more efficient) over eigendecomposition

Principal Component Analysis

Example: Iris Dataset

2. Eigenvectors and eigenvalues

$$\Sigma = \begin{bmatrix} 1.0067 & -0.1101 & 0.8776 & 0.8234 \\ -0.1101 & 1.0067 & -0.4233 & -0.3589 \\ 0.8776 & -0.4233 & 1.0067 & 0.9692 \\ 0.8234 & -0.3589 & 0.9692 & 1.0067 \end{bmatrix}$$

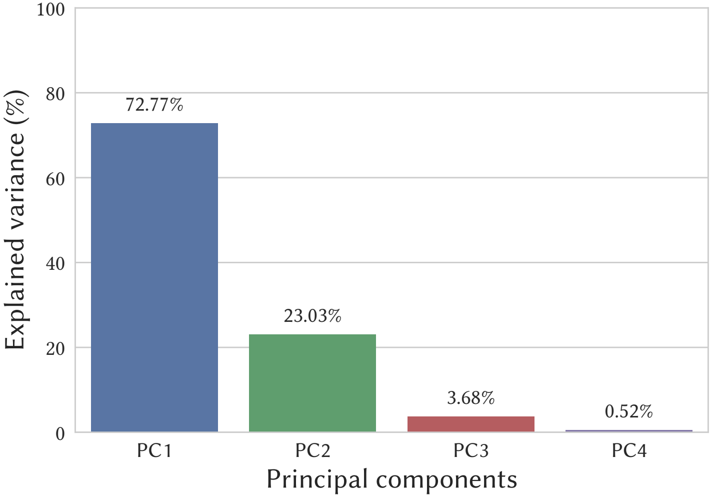
$$V = \begin{bmatrix} 0.5224 & -0.3723 & -0.7210 & 0.2620 \\ -0.2634 & -0.9256 & 0.2420 & -0.1241 \\ 0.5813 & -0.0211 & 0.1409 & -0.8012 \\ 0.5656 & -0.0654 & 0.6338 & 0.5235 \end{bmatrix}, \lambda = \begin{bmatrix} 2.9304 \\ 0.9274 \\ 0.1483 \\ 0.0207 \end{bmatrix}^T$$

- Four dimensions $\rightarrow$ four eigen vector/value pairs
- Lamba values represent the amount of variance explained by each principal component

Principal Component Analysis

Example: Iris Dataset

3. Choosing principal components (PC1 and PC2)



Principal Component Analysis

Example: Iris Dataset

4. Construct the projection matrix
   - We keep the first two *eigenvectors* corresponding to the two principal components, and we obtain

$$\mathbf{W} = \begin{bmatrix} 0.5224 & -0.3723 \\ -0.2634 & -0.9256 \\ 0.5813 & -0.0211 \\ 0.5656 & -0.0654 \end{bmatrix}$$

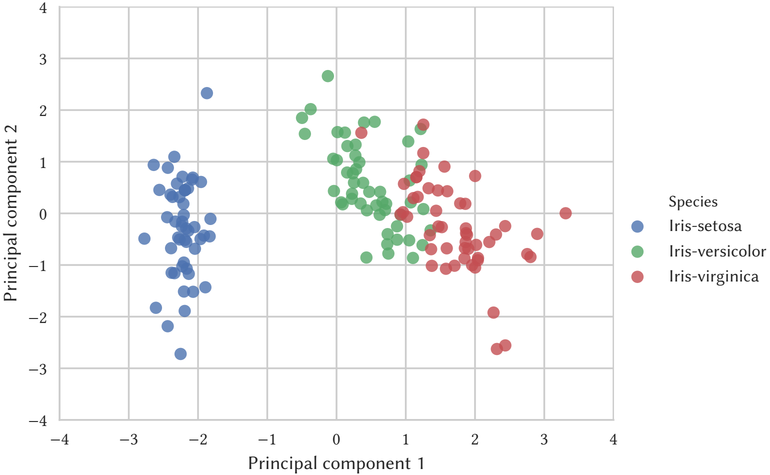
5. Project the feature space

$$\mathbf{Y} = \mathbf{X}\mathbf{W}$$

Principal Component Analysis

Example: Iris Dataset

Samples scatterplot in the lower-dimensional feature space



Principal Component Analysis

Example: Iris Dataset

Contribution of original features to each principal component

	Principal component 1	Principal component 2
Sepal length	79.43%	12.77%
Sepal width	20.19%	78.92%
Petal length	98.34%	0.04%
Petal width	93.12%	0.39%