PRINCIPAL COMPONENTS ANALYSIS

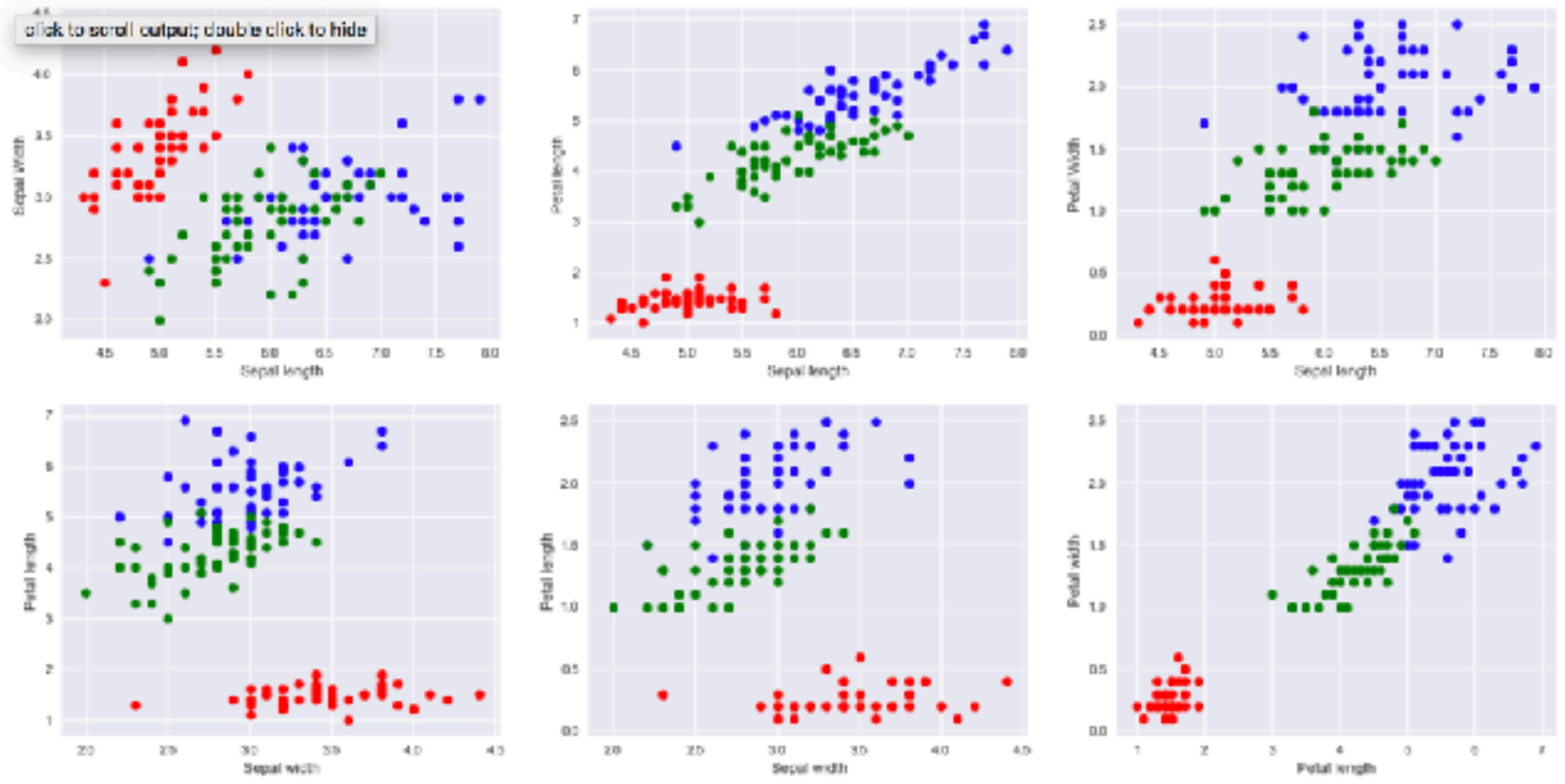
PCA - INTRODUCTION

$$X = \begin{bmatrix} 1 & 2 & 4 \\ 2 & 1 & 5 \\ 3 & 4 & 10 \\ 4 & 3 & 11 \end{bmatrix}$$

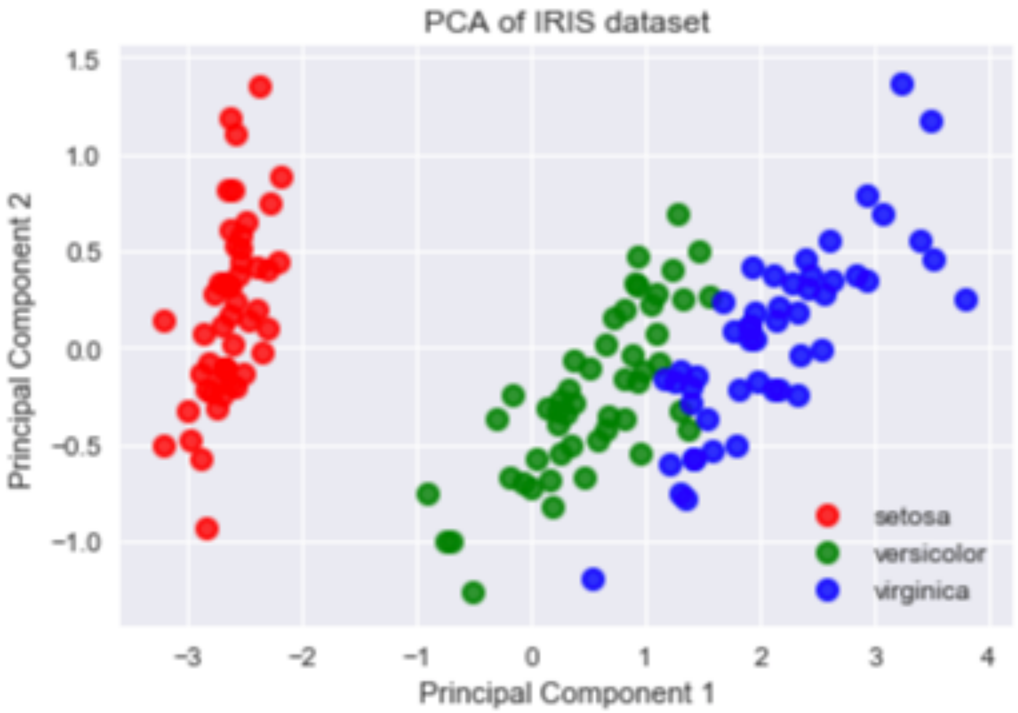
PCA - INTRODUCTION

	sepal_length	sepal_width	petal_length	petal_width	species
8	4.4	2.9	1.4	0.2	setosa
52	6.9	3.1	4.9	1.5	versicolor
35	5.0	3.2	1.2	0.2	setosa
127	6.1	3.0	4.9	1.8	virginica
96	5.7	2.9	4.2	1.3	versicolor

PCA - INTRODUCTION



PCA - INTRODUCTION



PRINCIPAL COMPONENT ANALYSIS

- A technique to find the directions along which the points (set of tuples) in high-dimensional data line up best.
- Treat a set of tuples as a matrix M and find the eigenvectors for MM^T or M^TM.
- The matrix of these eigenvectors can be thought of as a rigid rotation in a high-dimensional space.
- When this transformation is applied to the original data - the axis corresponding to the principal eigenvector is the one along which the points are most “spread out”.

PRINCIPAL COMPONENT ANALYSIS

- **When this transformation is applied to the original data - the axis corresponding to the principal eigenvector is the one along which the points are most "spread out".**
- **This axis is the one along which variance of the data is maximized.**
- **Points can best be viewed as lying along this axis with small deviations from this axis.**
- **Likewise, the axis corresponding the second eigenvector is the axis along which the variance of distances from the first axis is greatest, and so on.**

PRINCIPAL COMPONENT ANALYSIS

- Principal Component Analysis (PCA) is a dimensionality reduction method.

- The goal is to embed data in high dimensional space, onto a small number of dimensions.

- It most frequent use is in exploratory data analysis and visualization.

- It can also be helpful in regression (linear or logistic) where we can transform input variables into a smaller number of predictors for modeling.

PRINCIPAL COMPONENT ANALYSIS

- **Mathematically,**

  Given: Data set $\{x_1, x_2, \ldots, x_n\}$

  where, x_i **is the vector of p variable values for the i-th observation.**

  Return:

  Matrix $[\phi_1, \phi_2, \ldots, \phi_p]$

  of linear transformations that retain maximal variance.

- **You can think of the first vector** ϕ_1 **as a linear transformation that embeds observations into 1 dimension**

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p$$

PRINCIPAL COMPONENT ANALYSIS

- You can think of the first vector ϕ_1 as a linear transformation that embeds observations into 1 dimension

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \ldots + \phi_{p1}X_p$$

where ϕ_1 is selected so that the resulting dataset $\{z_i, \ldots, z_n\}$

has maximum variance.

- In order for this to make sense, mathematically, data has to be centered
  - Each X_i has zero mean
  - Transformation vector ϕ_1 has to be normalized, i.e., $\sum_{j=1}^{p} \phi_{j1}^2 = 1$

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- We can find ϕ_1 by solving an optimization problem:

$$\max_{\phi_{11},\phi_{21},\ldots,\phi_{p1}} \frac{1}{n} \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \text{ s.t. } \sum_{j=1}^{p} \phi_{j1}^2 = 1$$

Maximize variance but subject to normalization constraint.

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- **The second transformation, ϕ_2 is obtained similarly with the added constraint that ϕ_2 is orthogonal to ϕ_1**

- **Taken together $[\phi_1, \phi_2]$ define a pair of linear transformations of the data into 2 dimensional space**

$$Z_{n\times 2} = X_{n\times p}[\phi_1, \phi_2]_{p\times 2}$$

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- Each of the columns of the Z matrix are called Principal components.
- The units of the PCs are meaningless.
- In practice we may also scale X_j to have unit variance.
- In general if variables X_j are measured in different units(e.g., miles vs. liters vs. dollars), variables should be scaled to have unit variance.

SPECTRAL THEOREM

Using Spectral theorem

$$(X^T X)\phi = \lambda\phi$$

$$XX^T(X\phi) = \lambda(X\phi)$$

Conclusion:

The matrices XX^T and $X^T X$ share the same nonzero eigenvalues

To get an eigenvector of XX^T from $X^T X$ multiply ϕ on the left by X

Very powerful, particularly if number of observations, m, and the number of predictors, n, are drastically different in size.

For PCA: $Cov(X,X) = XX^T$

EXAMPLE - PCA

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

Eigen Values and Eigen Vectors?

EXAMPLE - PCA

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

From spectral theorem:

$$(X^T X)\phi = \lambda\phi$$

$$X^T X = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 1 & 4 & 3 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} = \begin{bmatrix} 30 & 28 \\ 28 & 30 \end{bmatrix}$$

EXAMPLE - PCA

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

From spectral theorem:

$$(X^T X)\phi = \lambda\phi \implies (X^T X)\phi - \lambda I\phi = 0$$

$$((X^T X) - \lambda I)\phi = 0$$

$$\begin{bmatrix} 30-\lambda & 28 \\ 28 & 30-\lambda \end{bmatrix} = 0 \implies \lambda = 58 \text{ and } \lambda = 2$$

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From spectral theorem:

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$$\begin{bmatrix} 30 & 28 \\ 28 & 30 \end{bmatrix} \begin{bmatrix} \phi_{21} \\ \phi_{22} \end{bmatrix} = 2 \begin{bmatrix} \phi_{21} \\ \phi_{22} \end{bmatrix} \implies \phi_2 = \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

EXAMPLE - PCA

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

From spectral theorem: $(X^T X)\phi = \lambda\phi$

$$\phi_1 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad \lambda_1 = 58 \qquad \phi_2 = \begin{bmatrix} \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \quad \lambda_2 = 2$$

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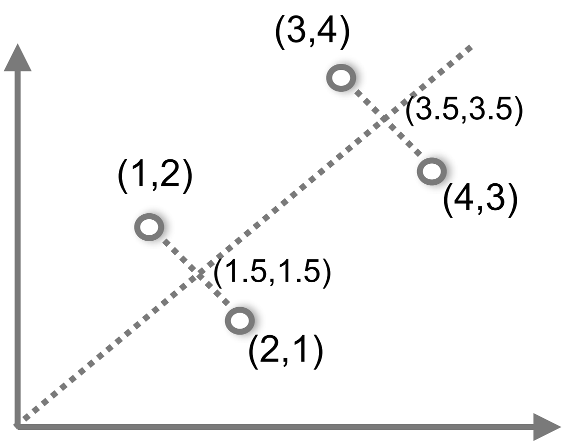
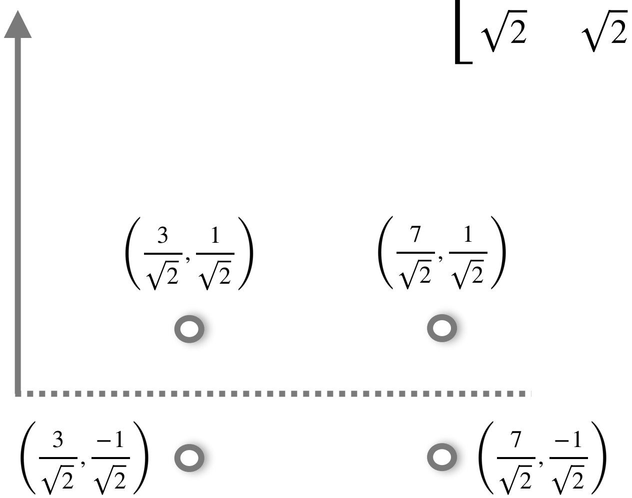
$$Z = X\phi = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} \frac{3}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{3}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \frac{7}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{7}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$

EXAMPLE - PCA

$$X = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ 3 & 4 \\ 4 & 3 \end{bmatrix}$$

$$Z = \begin{bmatrix} \frac{3}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{3}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ \frac{7}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{7}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$





HOW MANY PRINCIPAL COMPONENTS ?

- How many PCs should we consider in post-hoc analysis?
- One result of PCA is a measure of the variance to each PC relative to the total variance of the dataset.
- We can calculate the percentage of variance explained for the m-th PC:

$$PVE_m = \frac{\sum_{i=1}^{n} z_{im}^2}{\sum_{j=1}^{p} \sum_{i=1}^{n} x_{ij}^2}$$

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