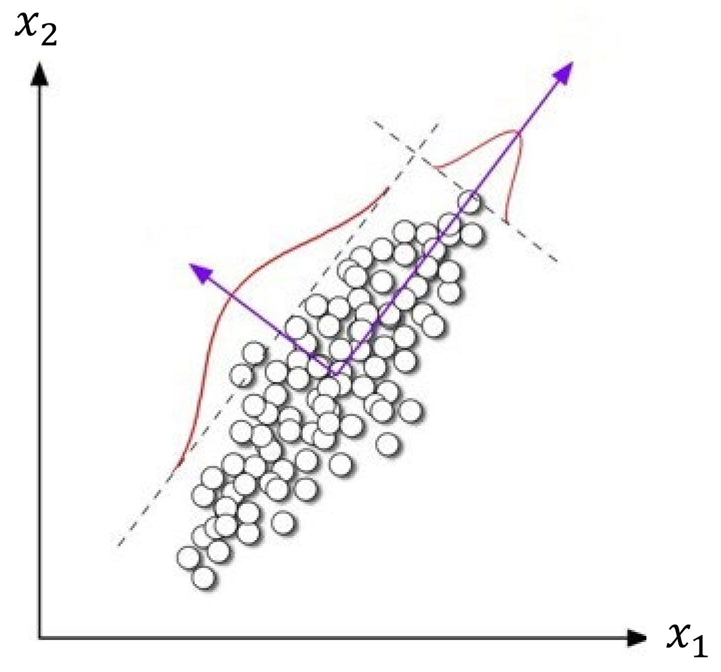
# Module 11
# Principal Component Analysis (PCA)

Prof. Pedram Jahangiry



# Class Modules

- Module 1- Introduction to Machine Learning
- Module 2- Setting up Machine Learning Environment
- Module 3- Linear Regression (Econometrics approach)
- Module 4- Machine Learning Fundamentals
- Module 5- Linear Regression (Machine Learning approach)
- Module 6- Penalized Regression (Ridge, LASSO, Elastic Net)
- Module 7- Logistic Regression
- Module 8- K-Nearest Neighbors (KNN)
- Module 9- Classification and Regression Trees (CART)
- Module 10- Bagging and Boosting
- **Module 11- Dimensionality Reduction (PCA)**
- Module 12- Clustering (KMeans – Hierarchical)

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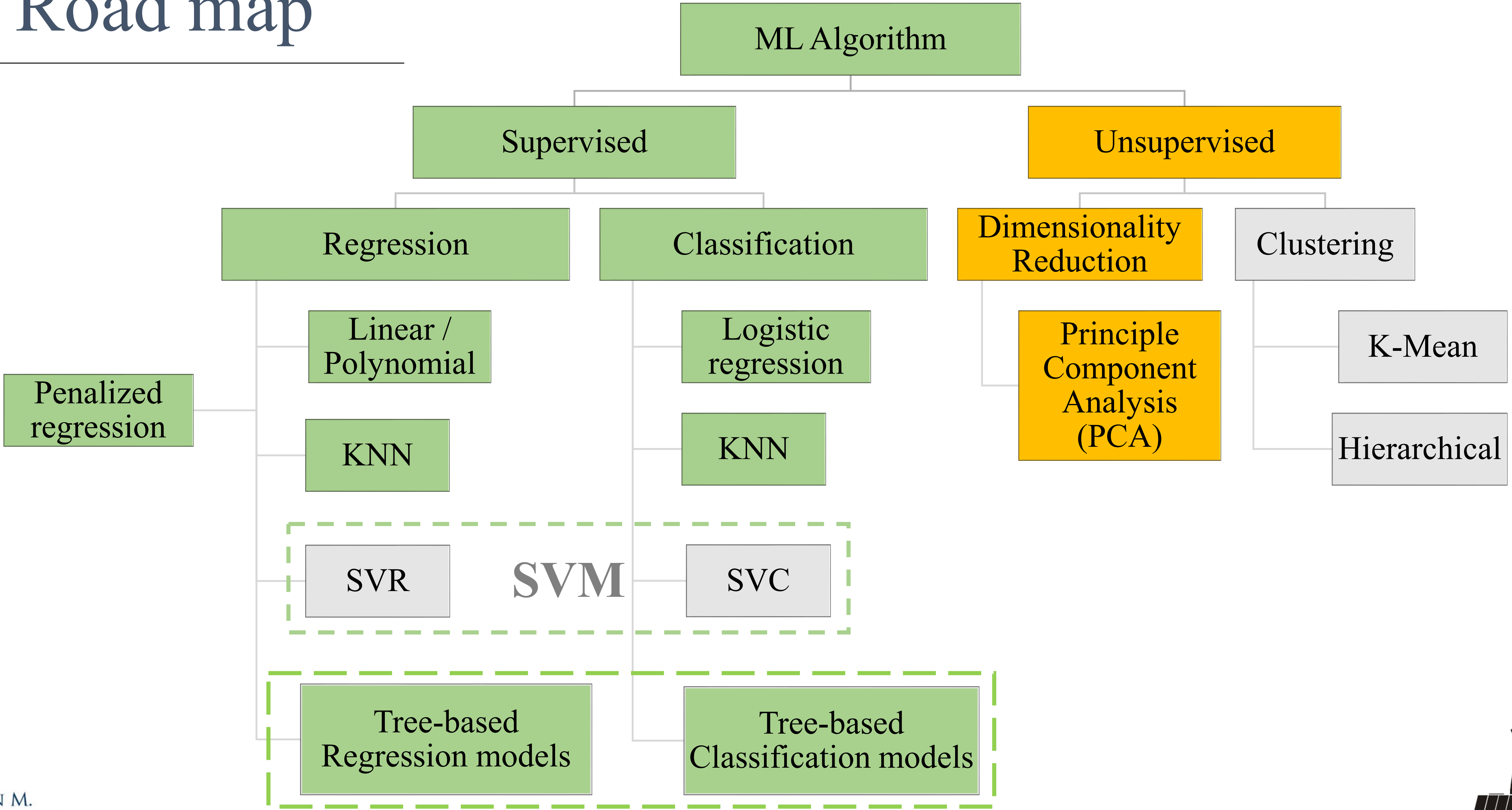
# Road map


ML Algorithm
Supervised
Unsupervised
Regression
Classification
Dimensionality Reduction
Clustering
Linear / Polynomial
Logistic regression
Principle Component Analysis (PCA)
K-Mean
Penalized regression
KNN
KNN
Hierarchical
SVR
SVM
SVC
Tree-based Regression models
Tree-based Classification models

# Topics

**Part I**

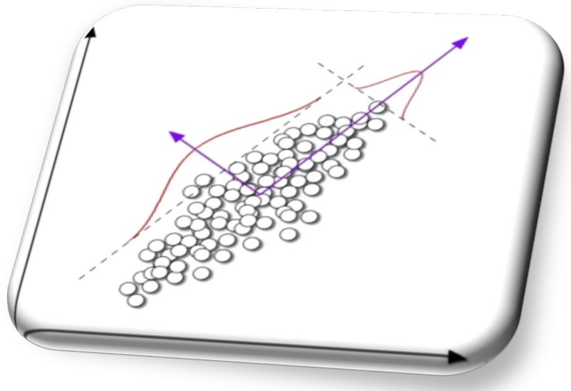
1. Unsupervised Machine Learning
2. Principal Component terminology

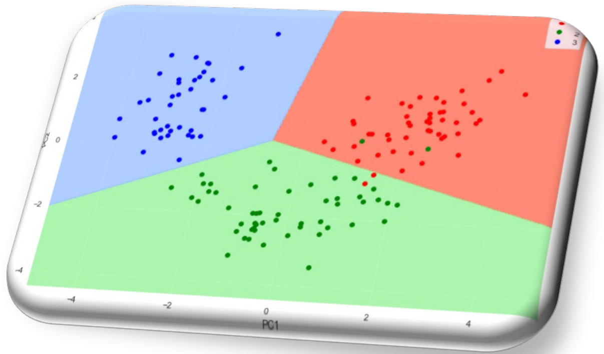
**Part II**

1. Principal Components Analysis (PC)
2. Scree plot

**Part III**

1. Why PCA? Pros and Cons!
2. Kernel PCA
3. Applications of PCA



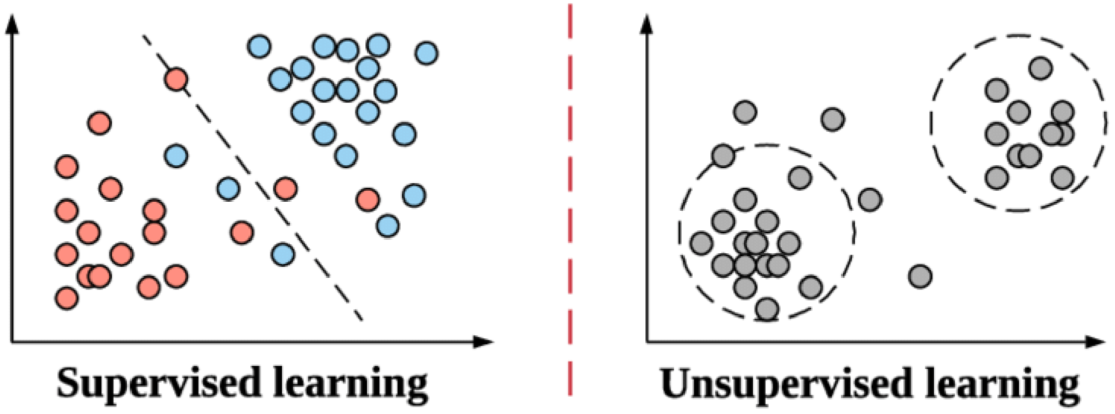


# Part I

1. Unsupervised Machine Learning
2. PC terminology

# Unsupervised Learning

- Unsupervised learning is a type of machine learning where the algorithm is not given any labeled training data.
- The goal is to discover the underlying patterns and find groups of samples that behave similarly. Find something interesting!
- The two main types of unsupervised learning algorithms are:
  1) Dimension reduction algorithm
     - Principal Component Analysis
  2) Clustering: group similar data
     - K-Mean
     - Hierarchical



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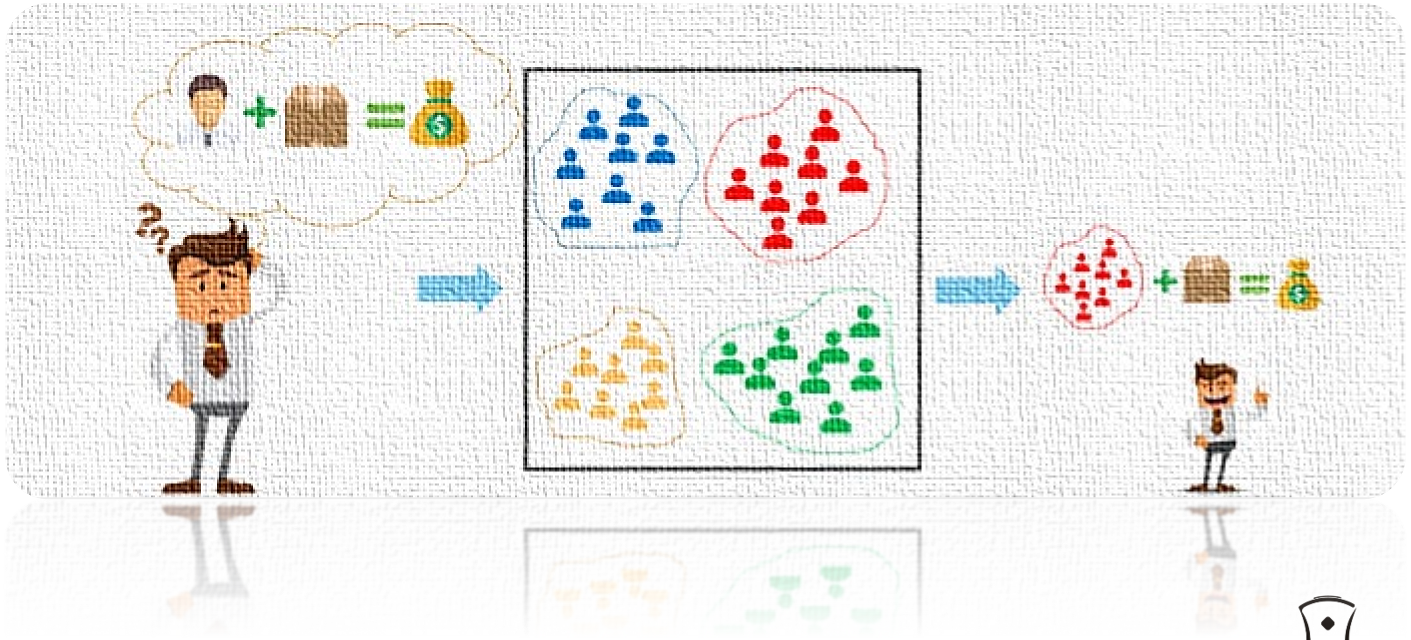
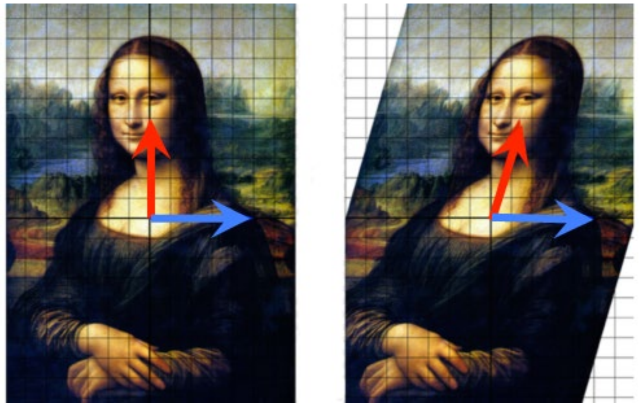
## Motivation

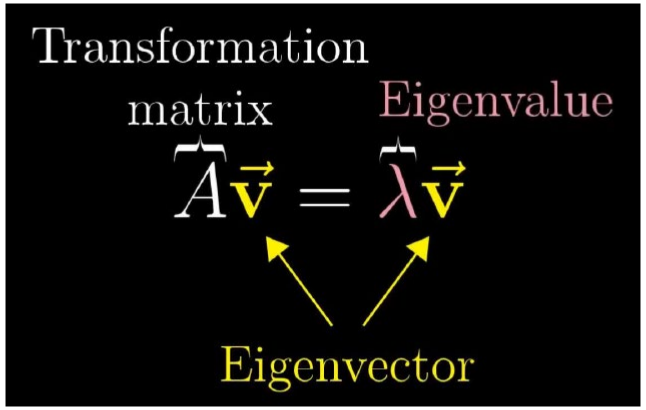
1) Dimension reduction algorithm: Principal Component Analysis
2) Clustering techniques: K-Mean for example



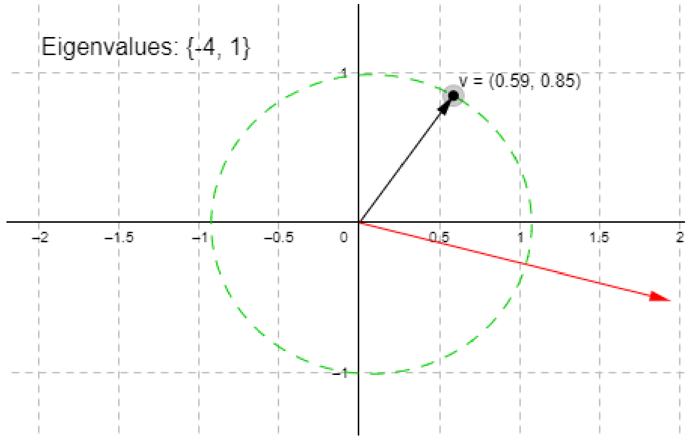
## Eigen things!

- Eigenvector does not change direction in a transformation.
- In this mapping, the blue arrow is eigenvector (why?)
- Its eigenvalue = 1 (why?)
- For a square matrix A, an Eigenvector and Eigenvalue are defined as follow:

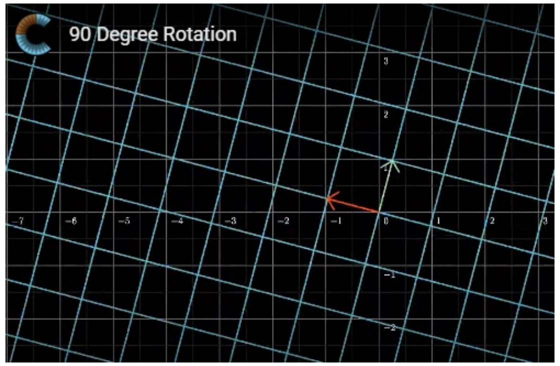




$$\overbrace{A}\vec{v} = \overbrace{\lambda}\vec{v}$$

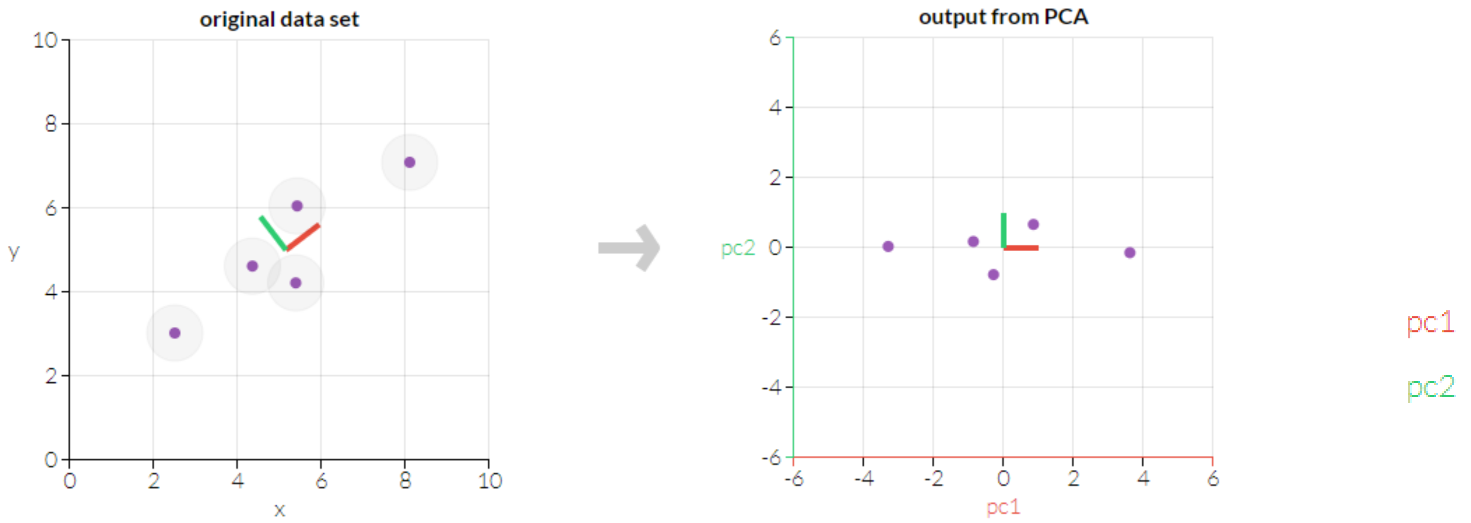


What is a transformation matrix?

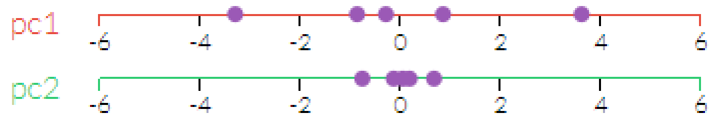


# PC terminology (connecting PC and Eigenthings)

- The eigenvectors and eigenvalues of a **covariance matrix** represent the "core" of a PCA
- Consider the following data points:



If you want to reduce the dimension of the data to 1, which PC would you drop?



- We want to find a direction(s) in the data set that explain the most variation. So, our transformation matrix will be the covariance matrix.
- The **principal components** (eigenvectors of the covariance matrix) determine the directions of the new feature space, and the eigenvalues determine their magnitude. In other words, the eigenvalues explain the variance of the data **along the new feature axes**.

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# PC terminology (PC definition)

In summary:

- Principal components are vectors that define a new coordinate system in which the first axis goes in the direction of the highest variance in the data.
- The second axis is orthogonal to the first one and goes in the direction of the second highest variance in the data.

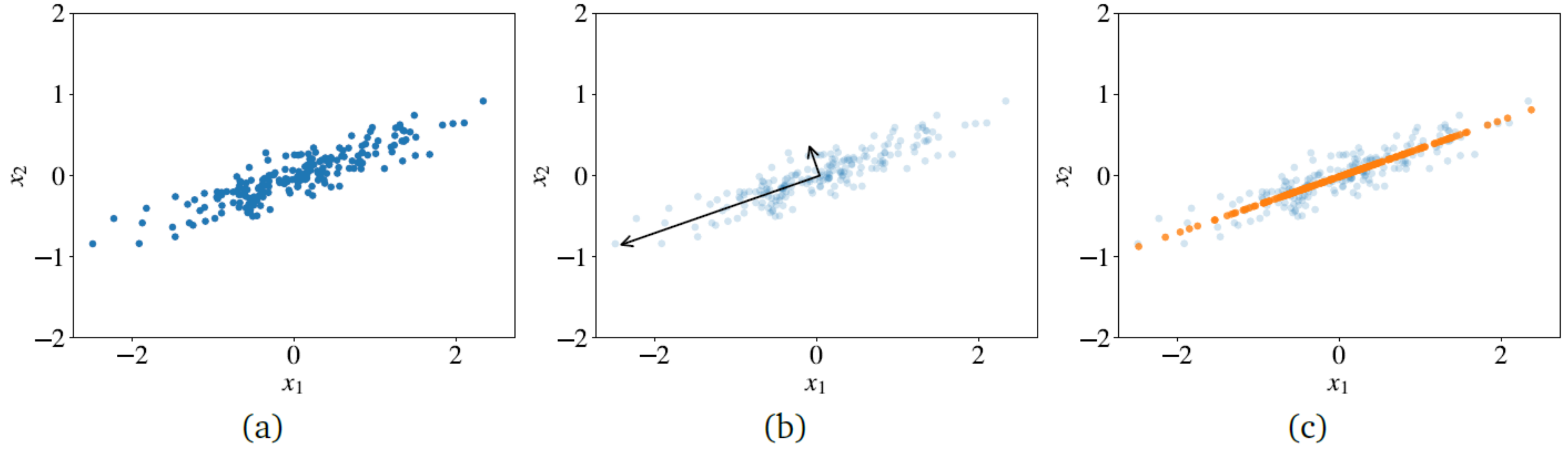
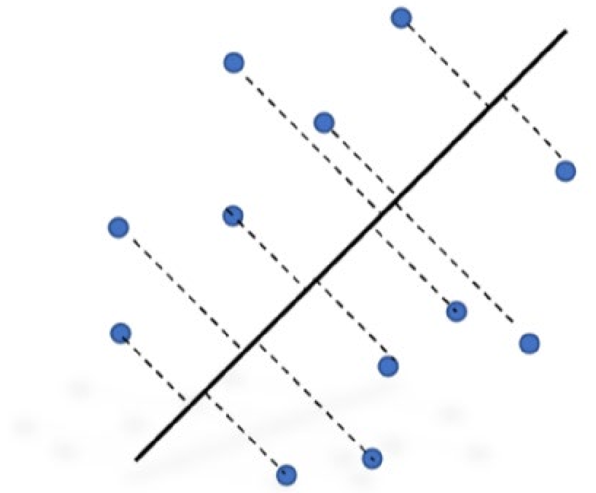
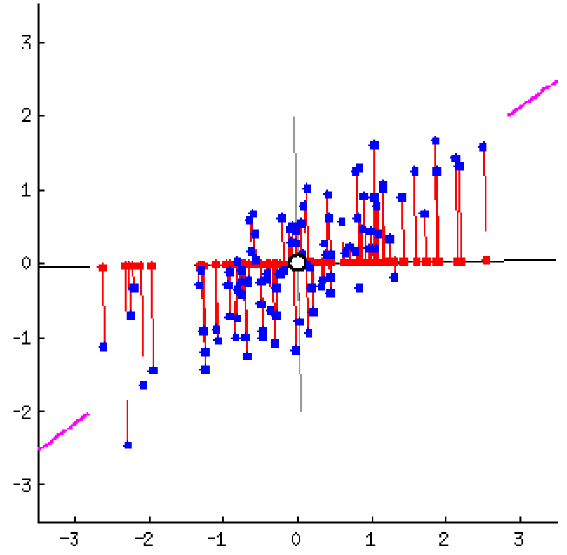


Figure 9.7: PCA: (a) the original data; (b) two principal components displayed as vectors; (c) the data projected on the first principal component. Source: The hundred-page machine learning book

## PC terminology (the objective function)

- Projection errors: The perpendicular distance (Euclidian) between the data point and a Principal Component.
- Spread: Variation of the data along Principal component.
- In PCA the goal is to minimize the projection errors (or equivalently maximize the spreads)



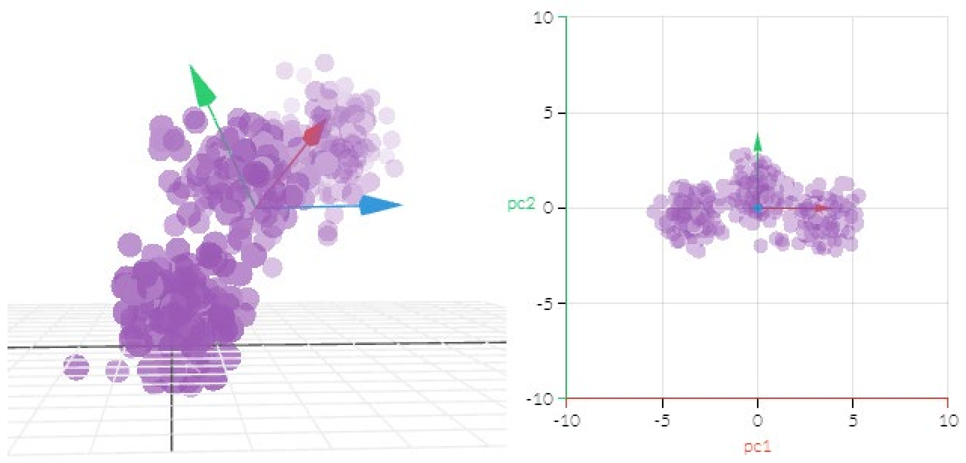


# Part II

1. Principal Component Analysis (PCA)
2. Proportion Variance Explained
3. Scree plot

# Principal Component Analysis (PCA)

- **Dimension reduction** aims to represent a dataset with many typically correlated features by a smaller set of features that still does well in describing the data.
- When many features in in a dataset, visualizing the data or fitting models to the data may become extremely complex and "noisy".
- Principal components analysis (PCA) is used to summarize or transform highly correlated features of data into a few main, uncorrelated components.
- The PCA algorithm orders the eigenvectors from highest to lowest according to their **usefulness** in explaining the **total variance** in the initial data (i.e., eigenvalues)



# PCA details

- The PC1 of a set of features $X_1, X_2, \dots, X_p$ is the normalized linear combination of the features that has the largest variance.

$$PC_1 = \phi_{11}X_1 + \phi_{21}X_2 + \dots + \phi_{p1}X_p \qquad \text{where } \sum_{j=1}^{p} \phi_{j1}^2 = 1$$

- The elements $\phi_{11}, \dots, \phi_{p1}$ are referred to as loadings of PC1.
- Note that the X features are standardized (why?)
- The loading vector $\phi_1$ defines a direction in feature space along which the data vary the most i.e., maximizing the variance in that direction!

$$\underset{\phi_{11},\dots,\phi_{p1}}{\text{maximize}} \frac{1}{n}\sum_{i=1}^{n}\left(\sum_{j=1}^{p}\phi_{j1}x_{ij}\right)^2 \text{ subject to } \sum_{j=1}^{p}\phi_{j1}^2 = 1$$

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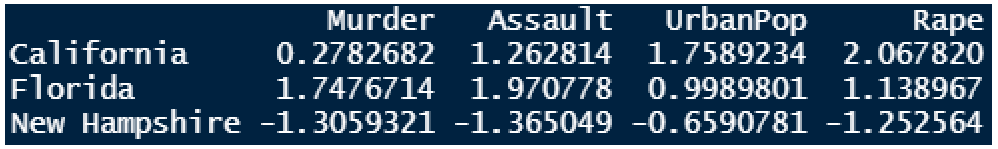
# USA arrests data: Biplot

- USA arrests data contains the number of arrests per 100k residents for each of the 50 states.
- The features are murder, assault, rape and urban population.
- PCA was performed after standardizing each feature! The loadings are as follow:

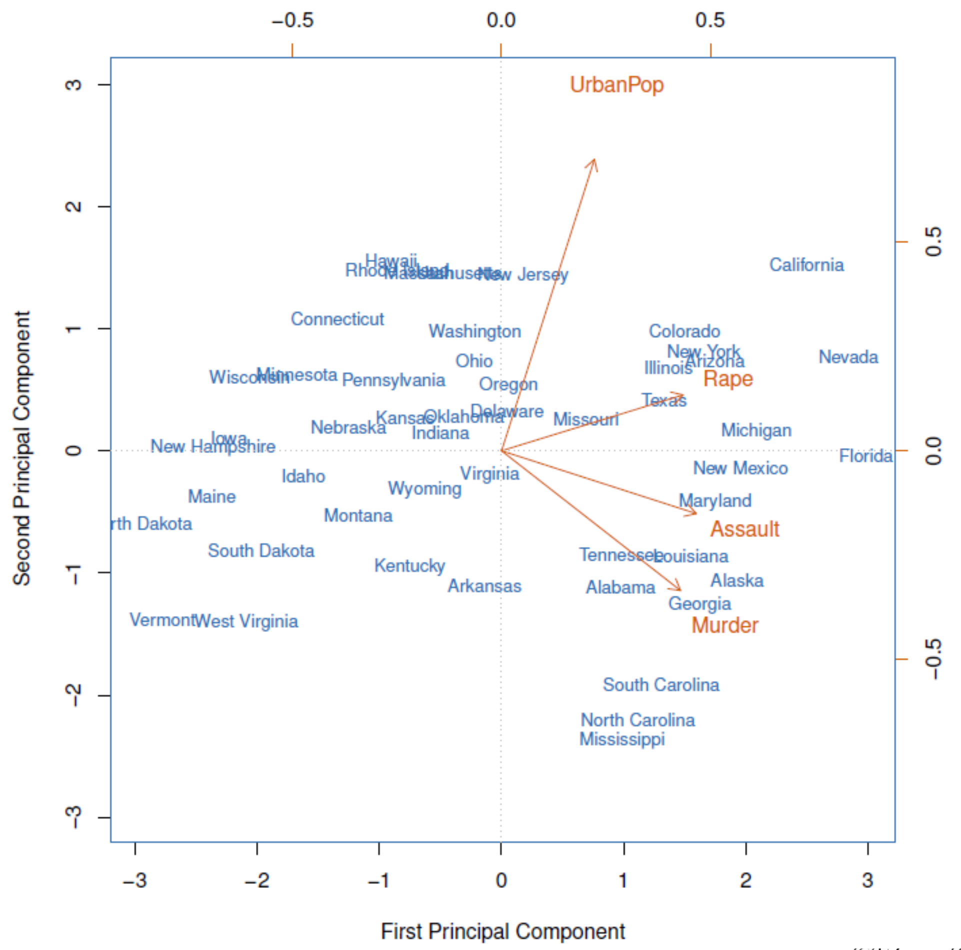
| | PC1 | PC2 |
|---|---|---|
| Murder | 0.5358995 | -0.4181809 |
| Assault | 0.5831836 | -0.1879856 |
| UrbanPop | 0.2781909 | 0.8728062 |
| Rape | 0.5434321 | 0.1673186 |

- Biplot displays both the PC scores and PC loadings.

Source: ISLR first edition



```
                 Murder   Assault   UrbanPop      Rape
California    0.2782682  1.262814  1.7589234  2.067820
Florida       1.7476714  1.970778  0.9989801  1.138967
New Hampshire -1.3059321 -1.365049 -0.6590781 -1.252564
```



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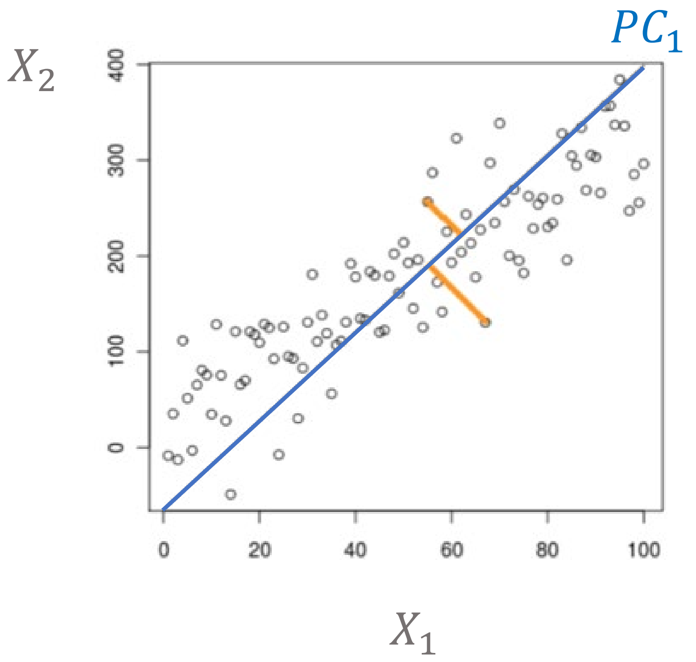
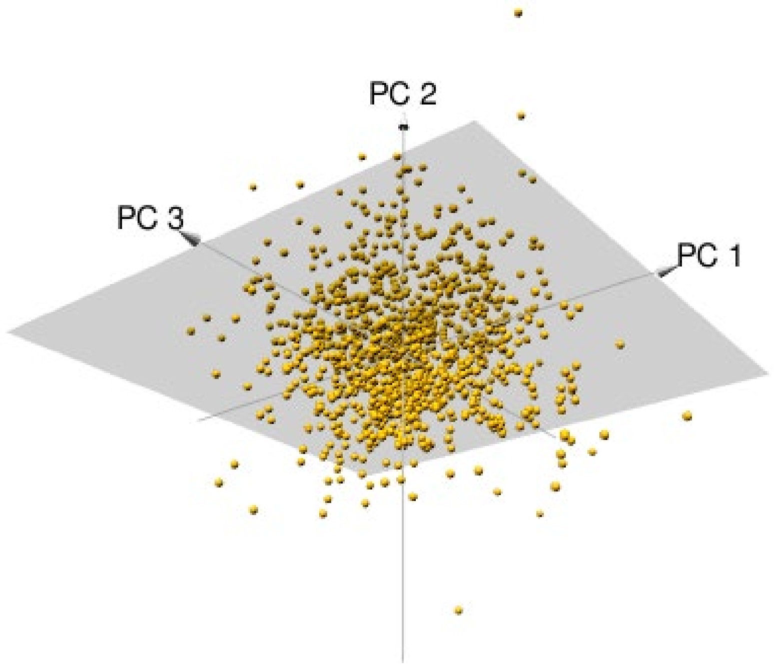
# Another interpretation of PCA

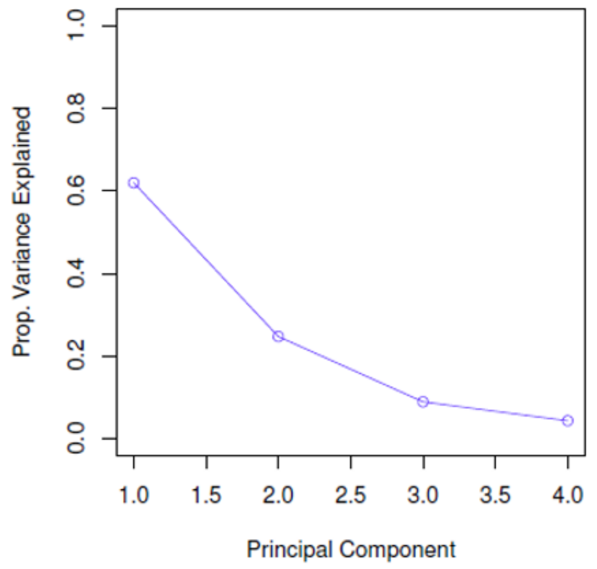
- PCA find the hyperplane closest to the observations!
- What is the difference between PCA and linear regression then?

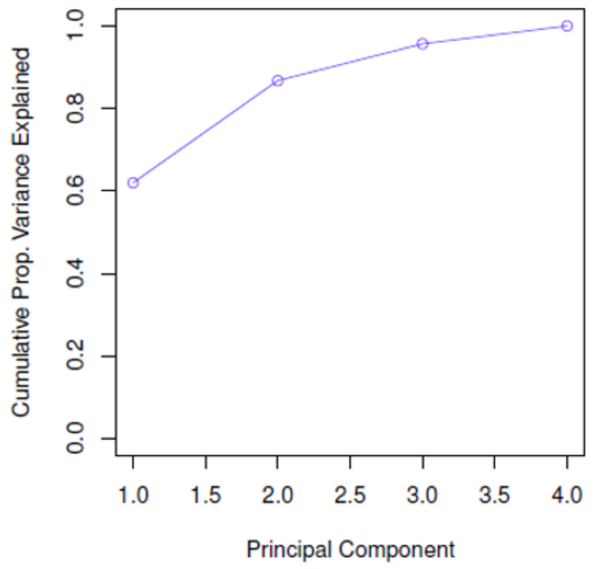




## Scree plot

- Scree plot shows the proportion of total variance in the data explained by each principal component. This is also called Proportion Variance Explained (PVE)
- The PVEs sum to one. Sometimes they are displayed as cumulative PVEs.





- What is the optimal number of PCs here?

# Part III

Why PCA? Pros and cons!

Kernel PCA

Applications of PCA

## PCA’s Pros and Cons

### Pros:

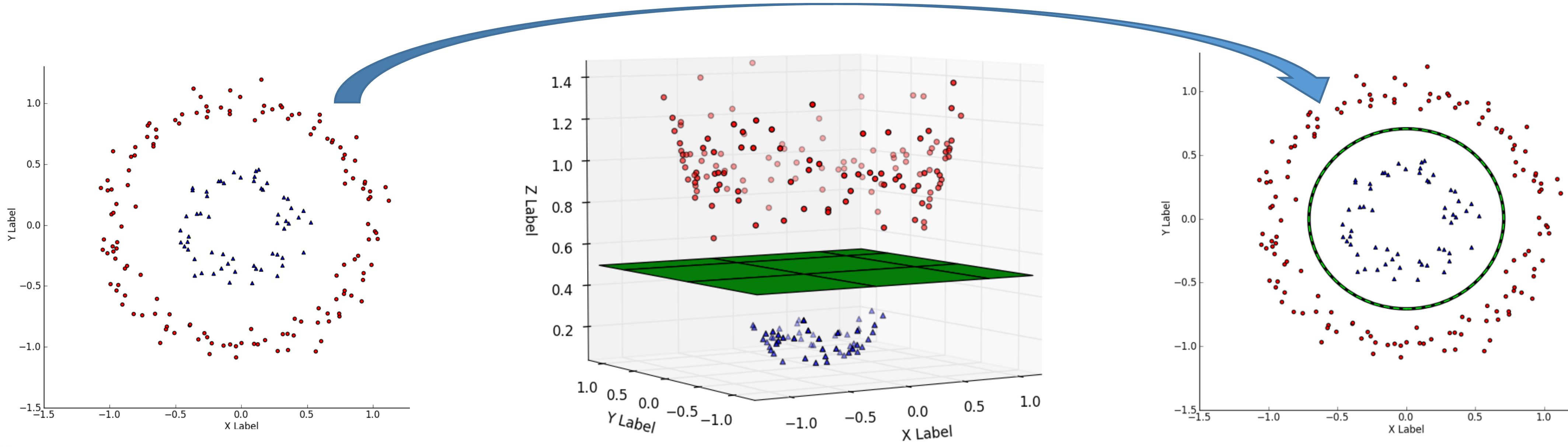
- Reducing the number of features to the most relevant predictors is very useful in general.
- Dimension reduction facilitates the data visualization in two or three dimensions.
- **Before** training another supervised or unsupervised learning model, it can be performed as part of EDA to identify patterns and detect correlations.
- Machine learning models are quicker to train, tend to reduce overfitting (by avoiding the curse of dimensionality), and are easier to visualized if provided with lower-dimensional datasets.

### Cons:

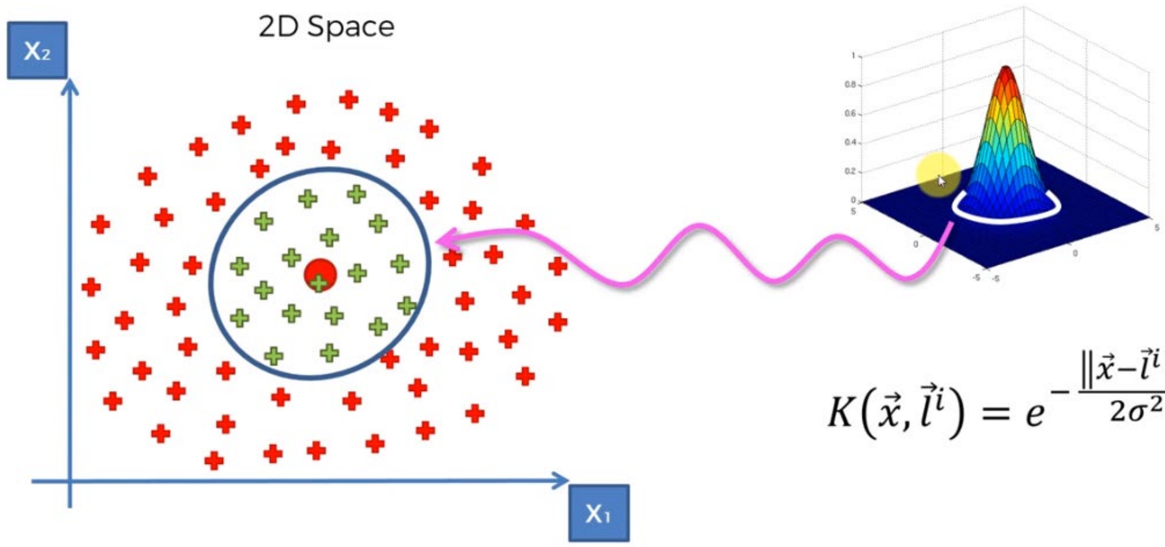
- Hard to interpret!
- Standard PCA is limited to linear transformations and may not capture the intrinsic structure of non-linear data.

## Kernel Trick!

- Non-linearly separable data
- We need a non-linear decision boundary!
- Mapping to higher dimensional space, finding the hyper plane and projecting it back to low dimensional space can be computationally expensive.
- Solution: Kernel Trick!



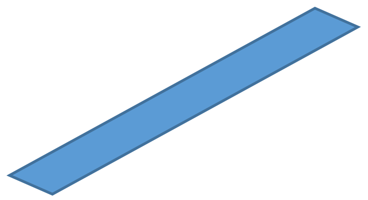
# The Gaussian RBF Kernel (Radial Basis Function)



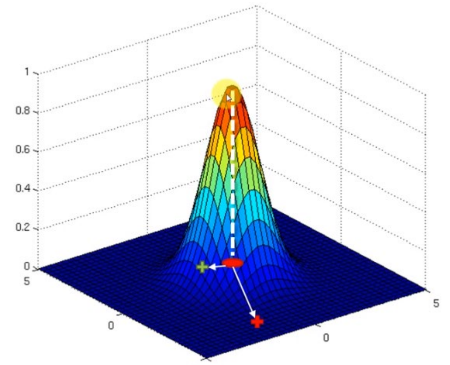
$$K(\vec{x}, \vec{l}^i) = e^{-\frac{\|\vec{x}-\vec{l}^i\|^2}{2\sigma^2}}$$

## Most common types of Kernel

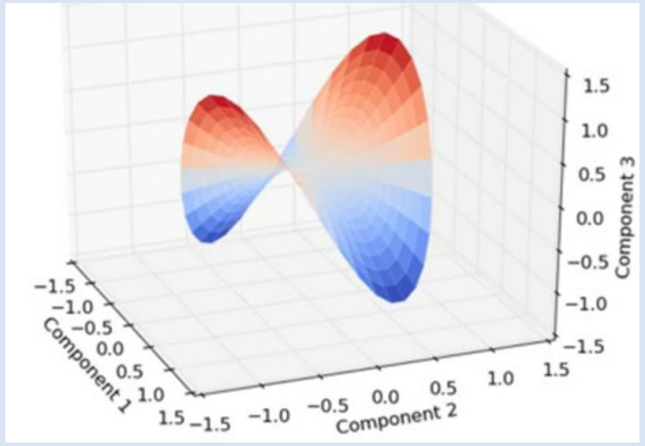
Linear Kernel



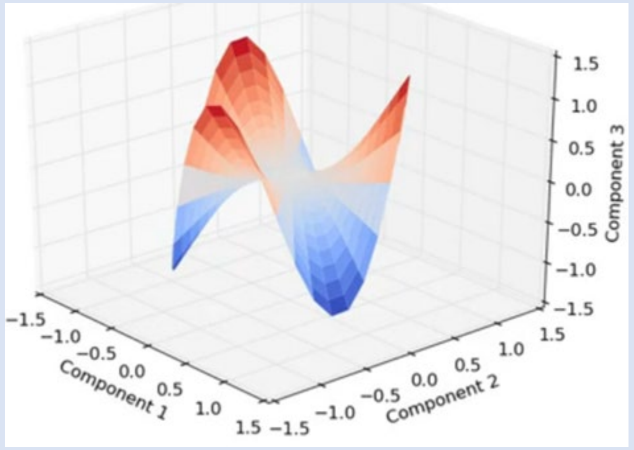
The Gaussian RBF Kernel



Polynomial Kernel

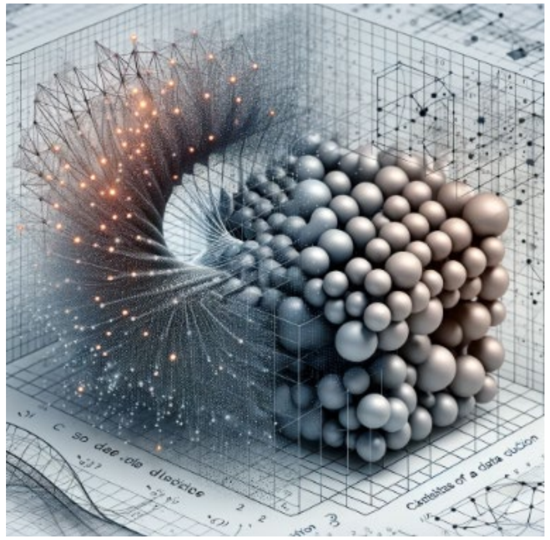


Sigmoid Kernel



# Kernel PCA

- Kernel PCA is an advanced form of PCA that utilizes kernel methods to enable effective dimensionality reduction in datasets with complex, non-linear structures.
- Process:
  - Kernel Transformation: Apply a kernel function (e.g., RBF, polynomial, sigmoid) to the original data, creating a kernel matrix that represents similarities between all data points.
  - Dimensionality Reduction: Perform PCA on the kernel matrix to extract principal components in the transformed feature space, capturing major variance in data according to non-linear relationships.



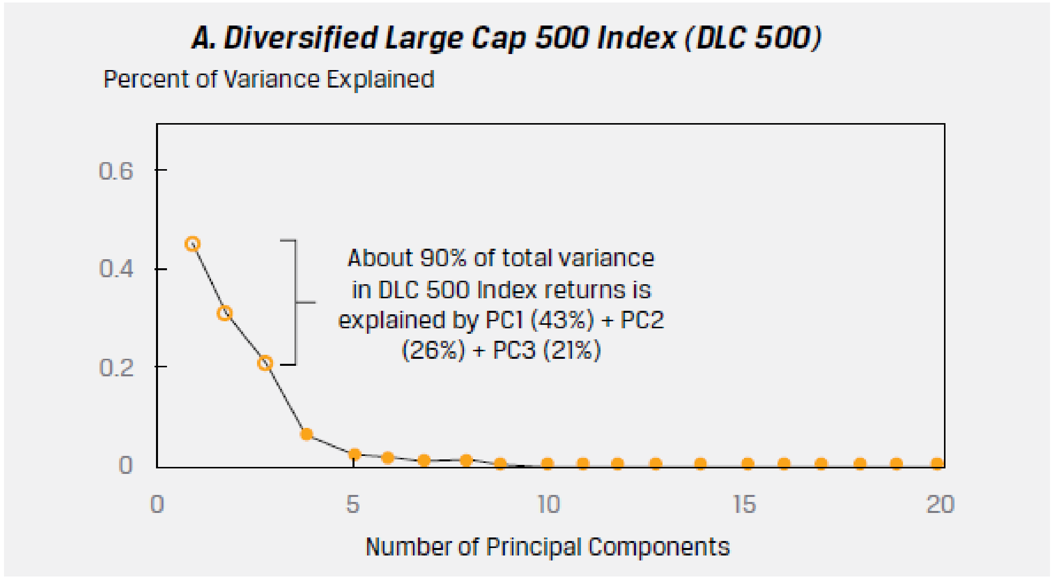
# Applications of PCA

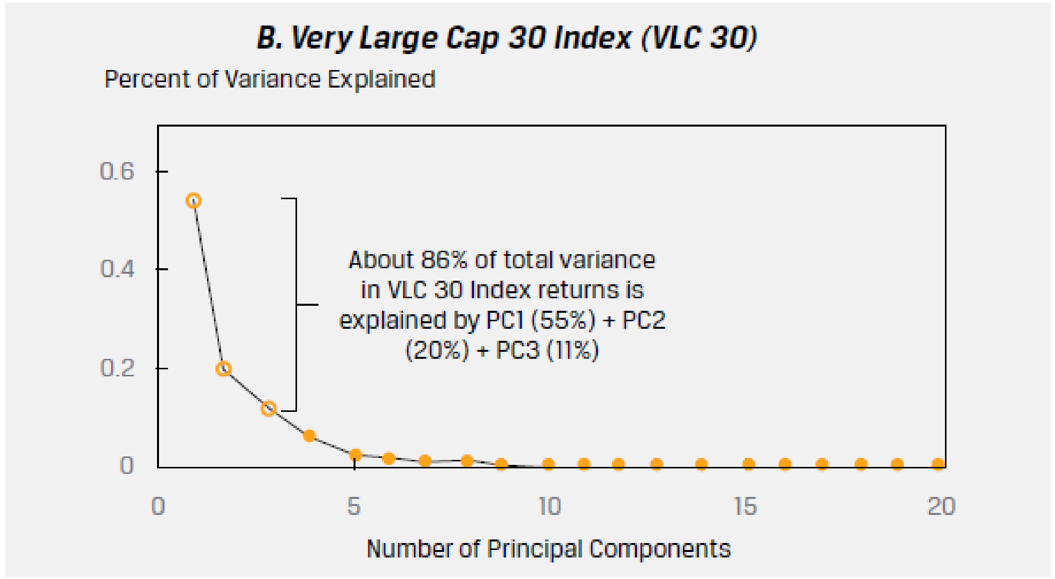
- Consider a hypothetical Diversified Large Cap (**DLC**) 500 and Very Large Cap (**VLC**) 30:
  - DLC 500 can be thought of as a diversified index of **500 large-cap companies** covering all economic sectors
  - VLC 30 is a more concentrated index of the **30 largest publicly traded companies**.

- The dataset consists of index prices and more than 2,000 fundamental and technical features
- Multi-collinearity among the features is inevitable!
- To mitigate the problem, PCA can be used to capture the information and variance in the data.

# Applications of PCA

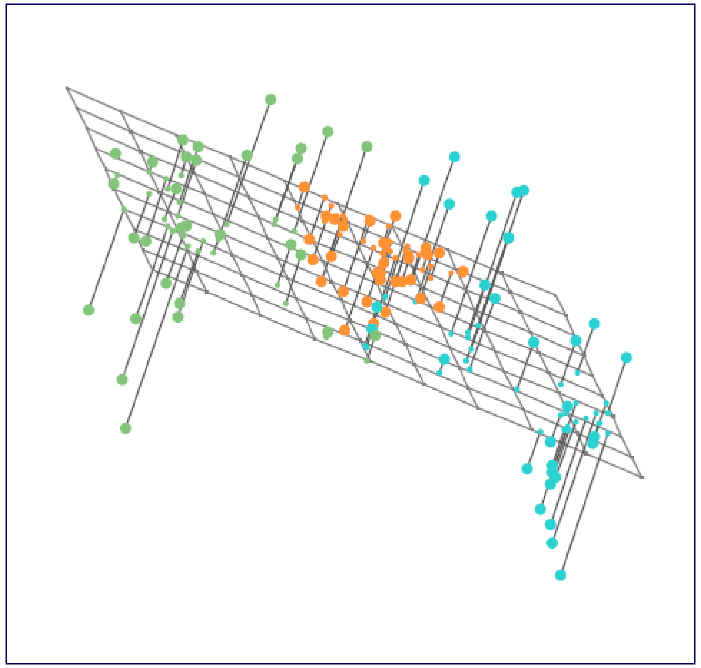
- The following scree plots show that of the 20 principal components generated, **the first 3 together** explain about 90% of the variance of DLC 500 and 86% of  the VLC 30.

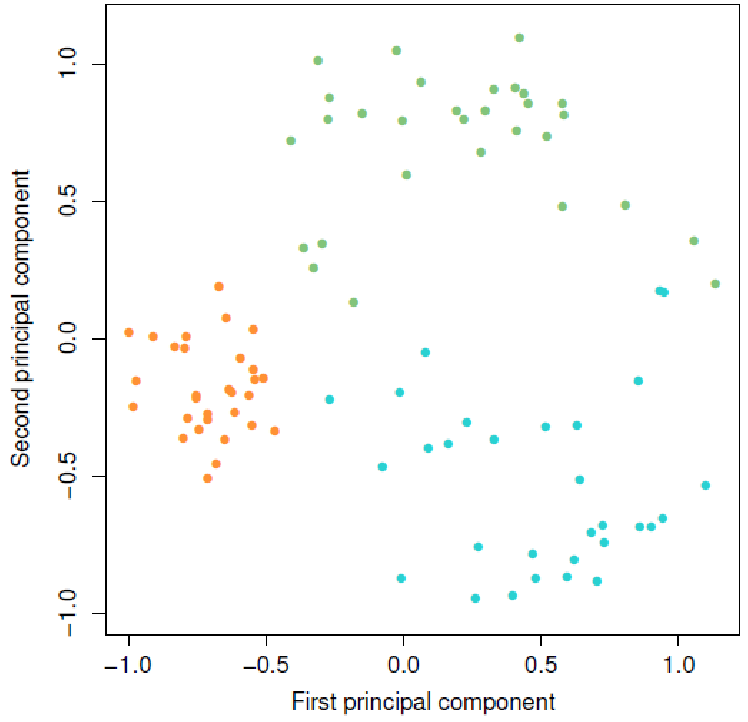




# Applications of PCA (Data visualization)

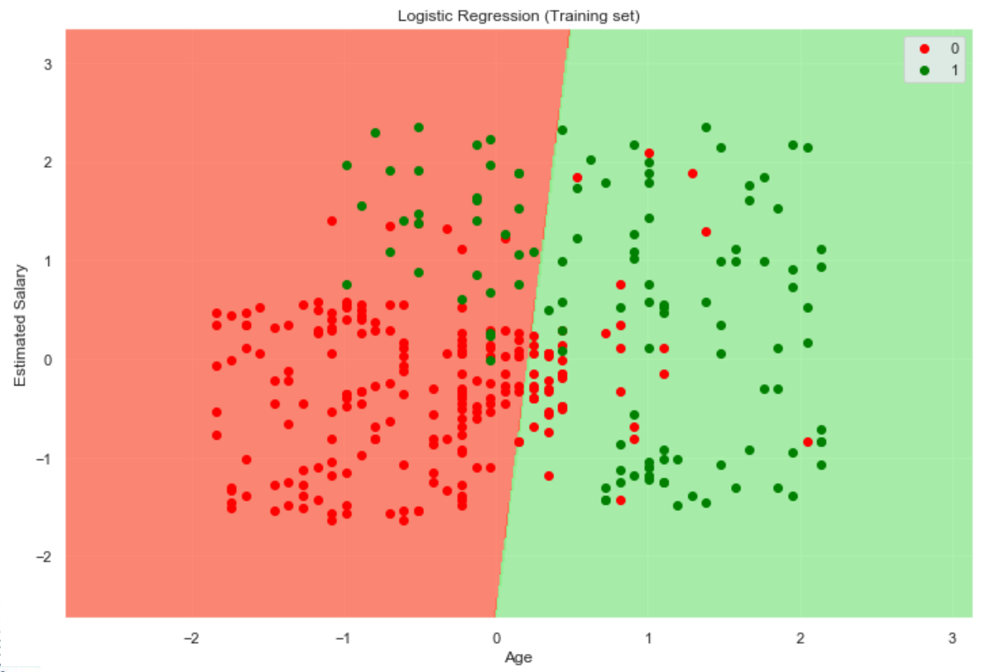
- PCA can be fed into other unsupervised or supervised learning models!
- Using PCA with an unsupervised model like K-Mean **clustering:**

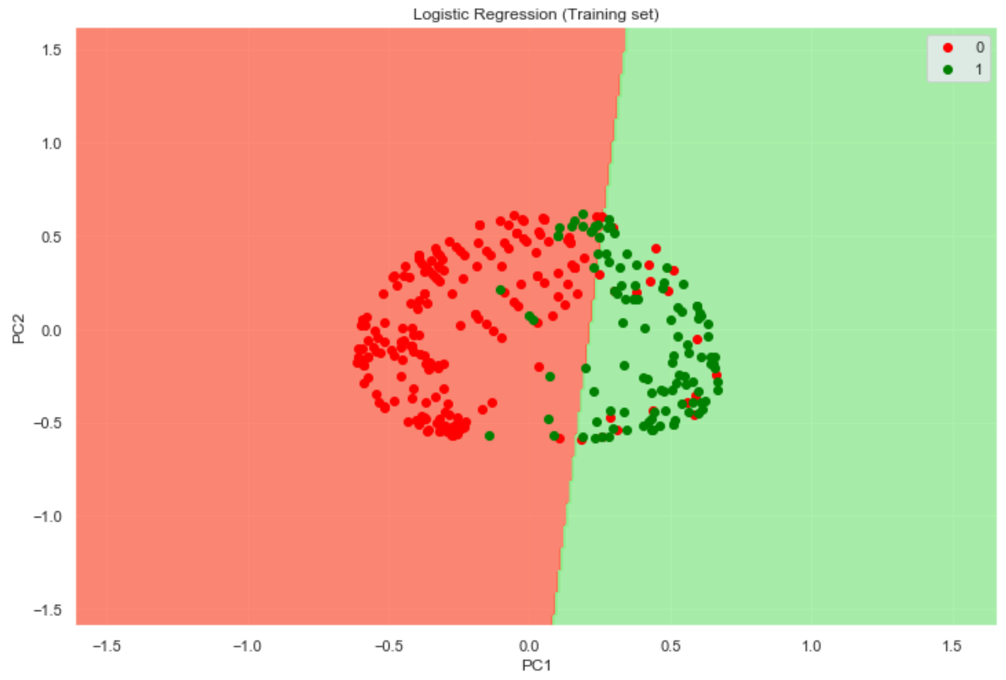




# Applications of PCA (Kernel PCA)

- What if we want to use a linear classifier (regressor) but the data is non-linearly separable?
- Solution: Kernel PCA
- Kernel PCA uses a kernel function to project dataset into a higher dimensional feature space, where it is linearly separable. (without explicitly going to higher dimensions)
- Using PCA with a supervised learning model like logistic regression:





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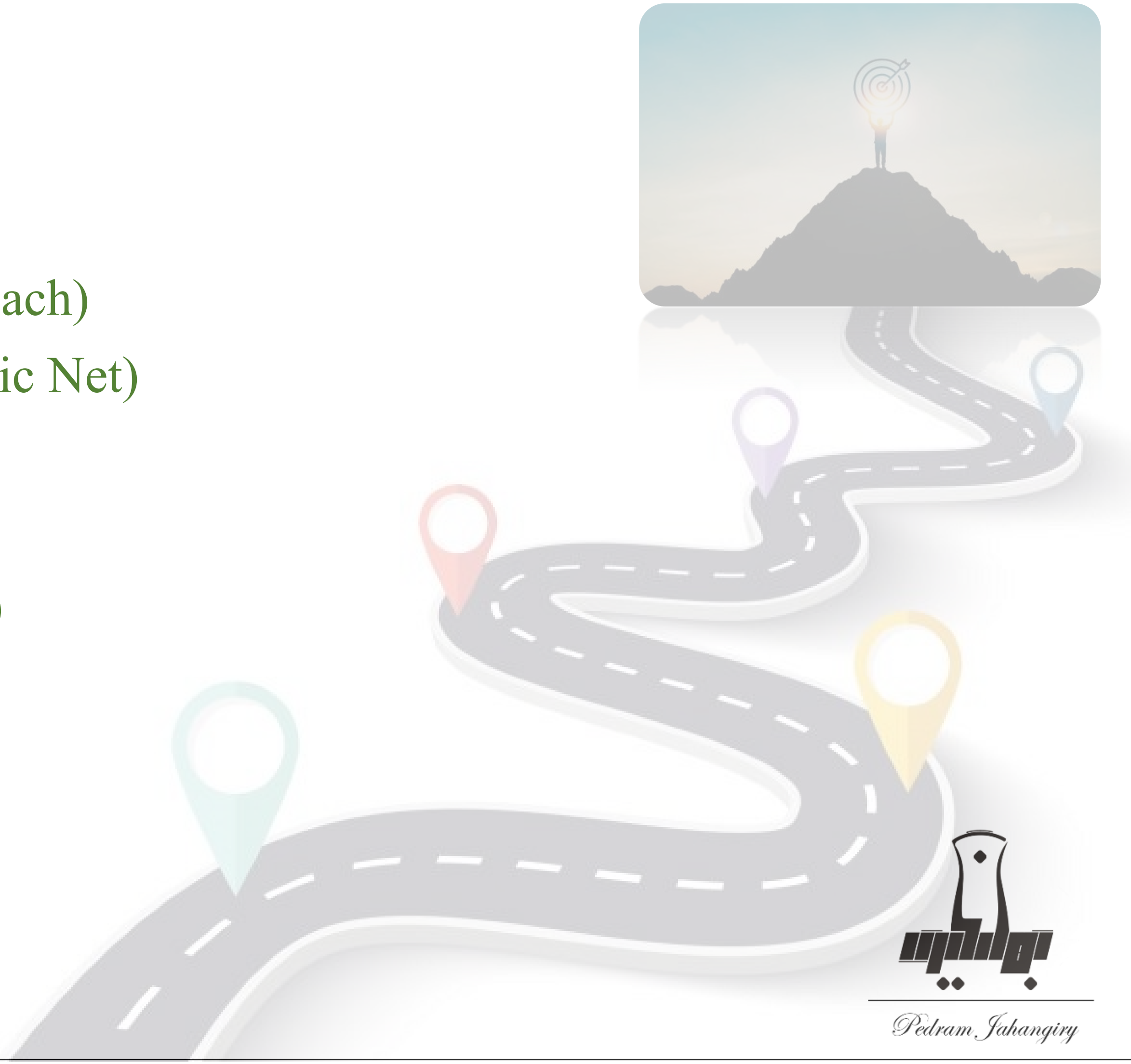

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