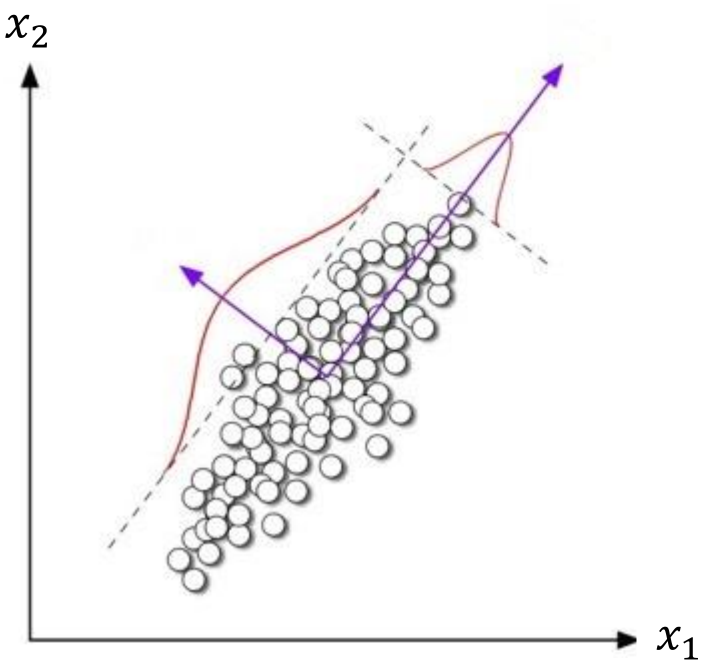
Class -23
Principal Component Analysis (PCA)

Prof. Pedram Jahangiry



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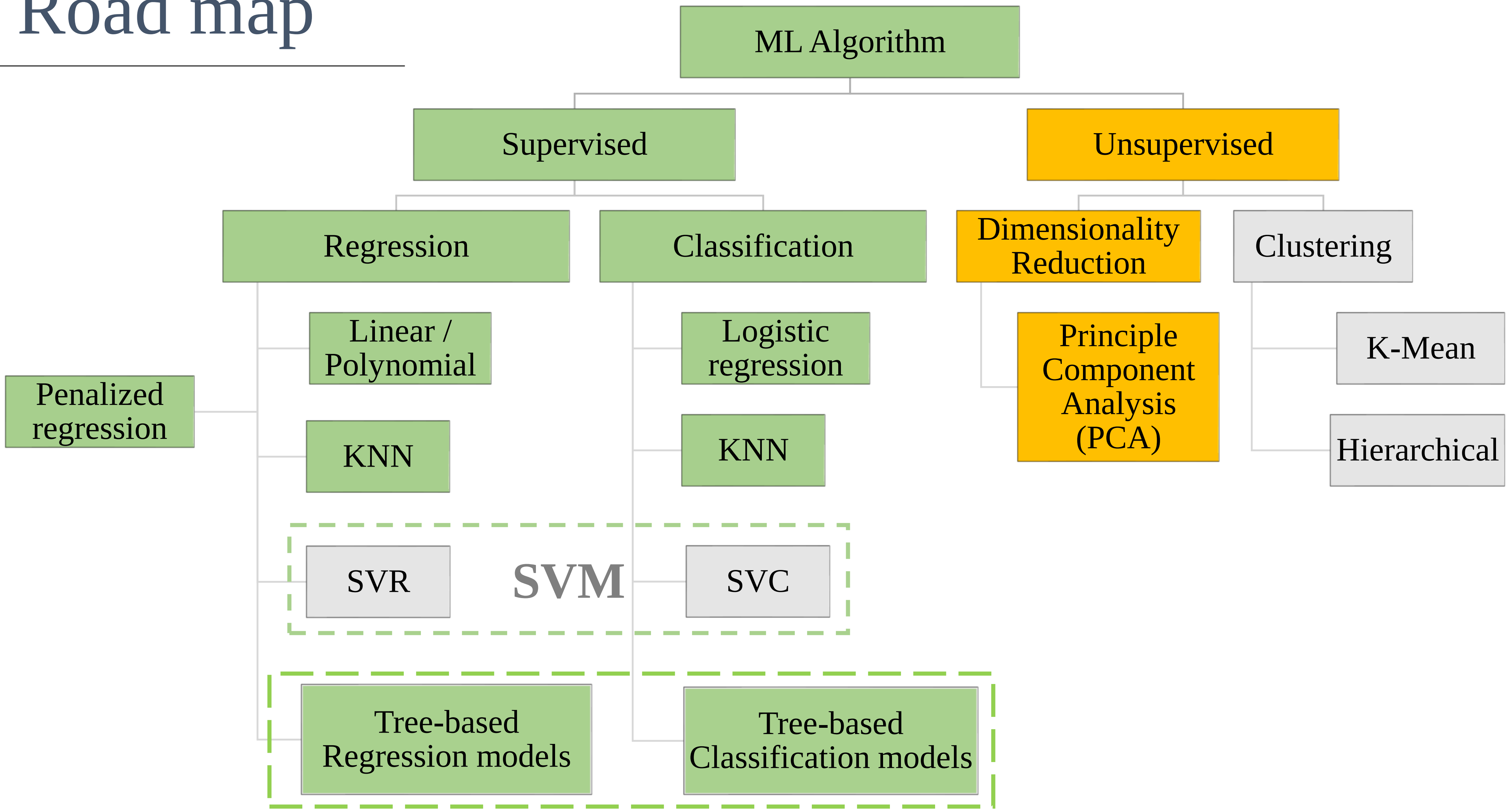
Road map



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

Topics

<u>Part I</u>

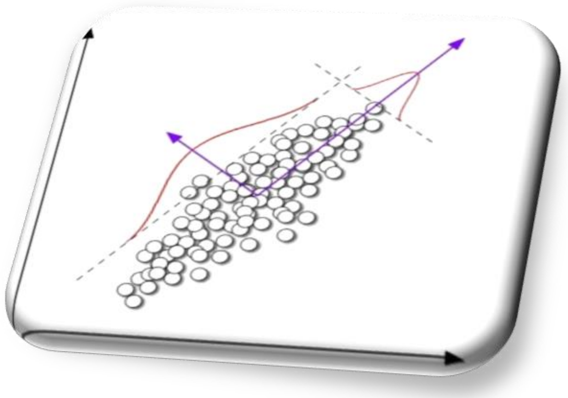
1. Unsupervised Machine Learning
2. Principal Component terminology

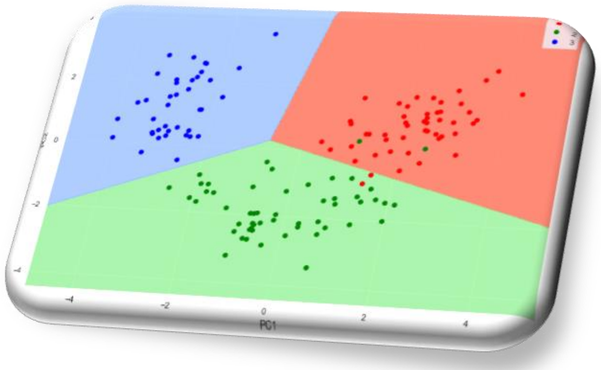
<u>Part II</u>

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

<u>Part III</u>

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



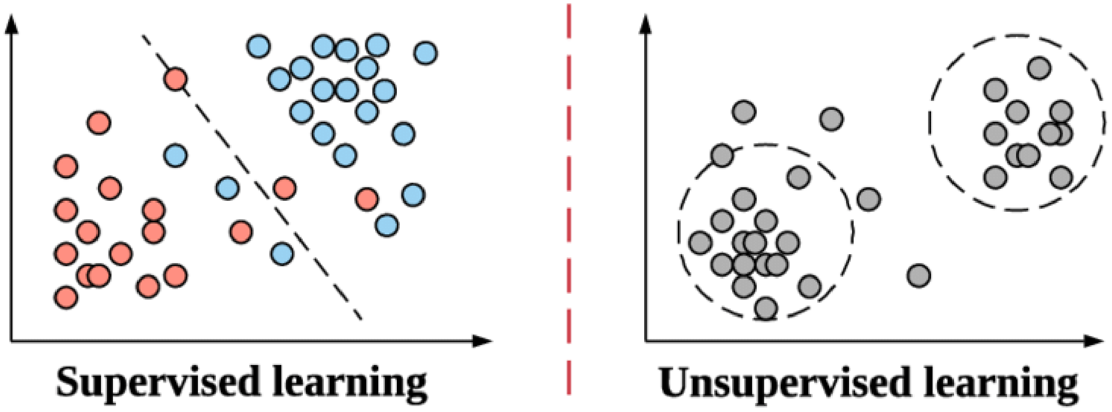


Part I

1. Unsupervised Machine Learning
2. PC terminology

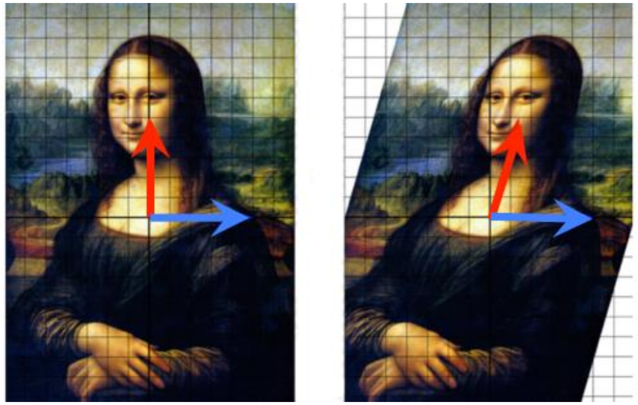
Unsupervised Learning

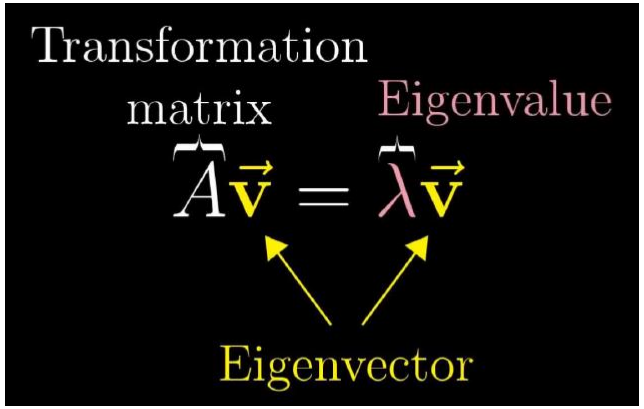
- Unsupervised learning is a machine learning technique that does not use labeled data (no target variable)
- The goal is to discover the underlying patterns and find groups of samples that behave similarly.
- The two main types of unsupervised learning algorithms are:
  1) Dimension reduction algorithm
     - Principal Component Analysis
  2) Clustering techniques
     - K-Mean
     - Hierarchical

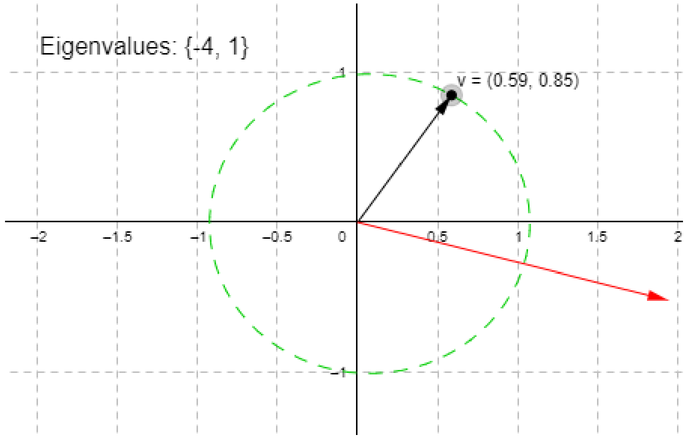


Eigen things!

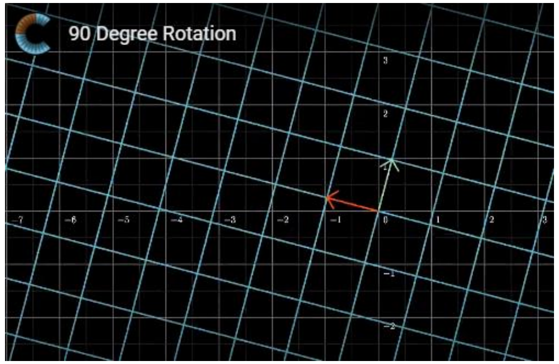
- Eigenvector does not change direction in a transformation.
- In this mapping, the blue arrow is eigenvector (why?)
- Its eigenvalue = 1 (why?)
- For a square matrix A, an Eigenvector and Eigenvalue are defined as follow:





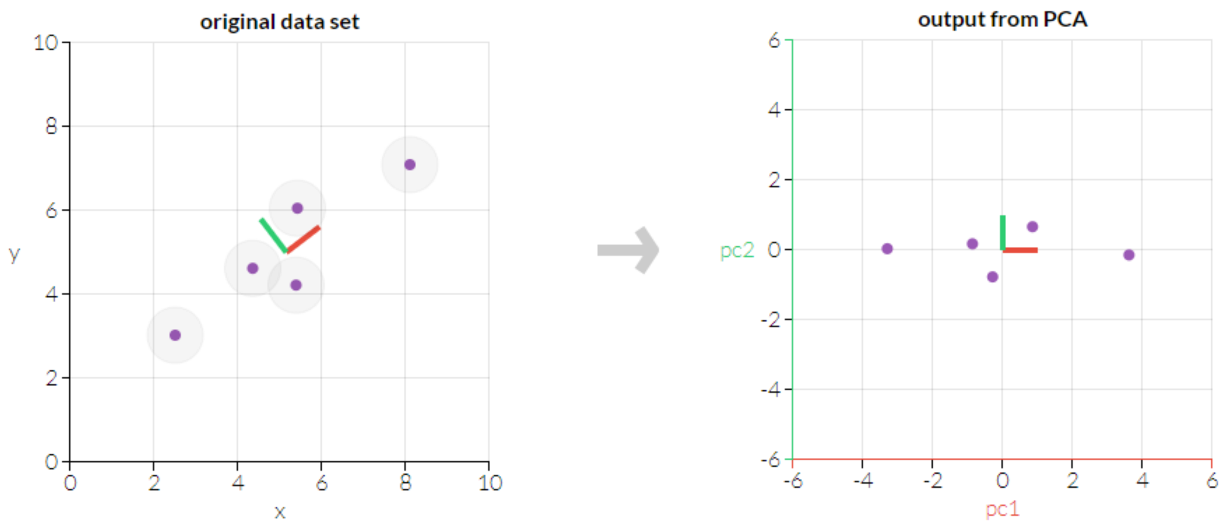


What is a transformation matrix?

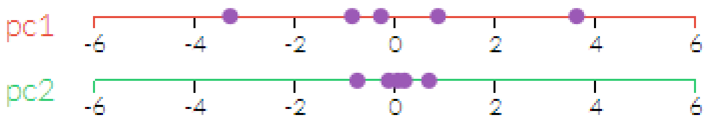


PC terminology (connecting PC and Eigenthings)

- 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**.

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.

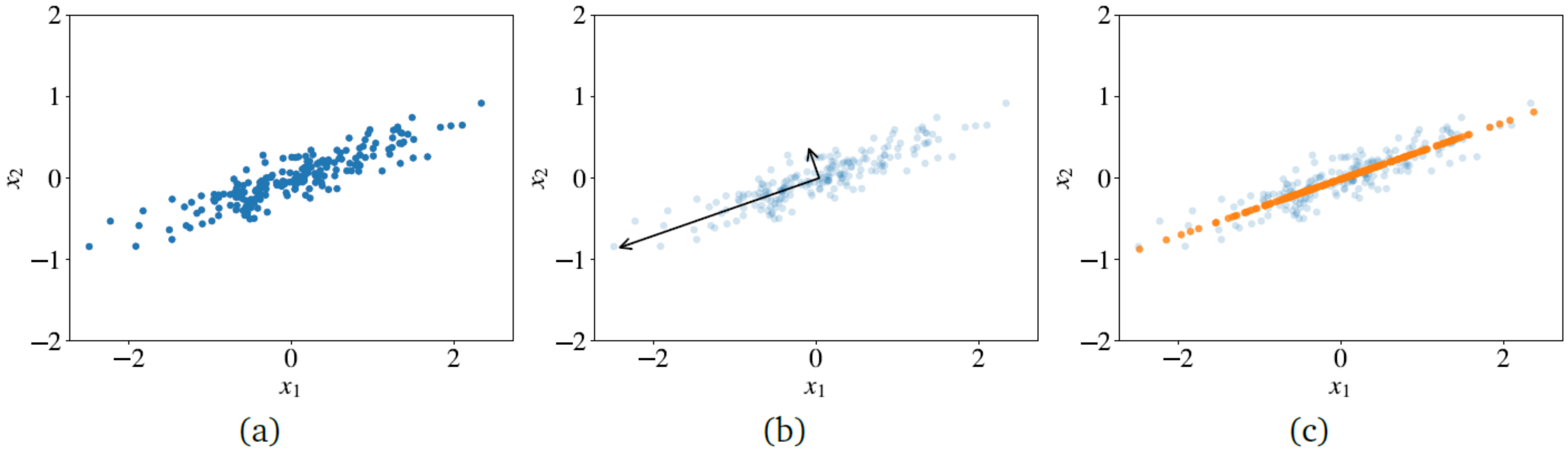
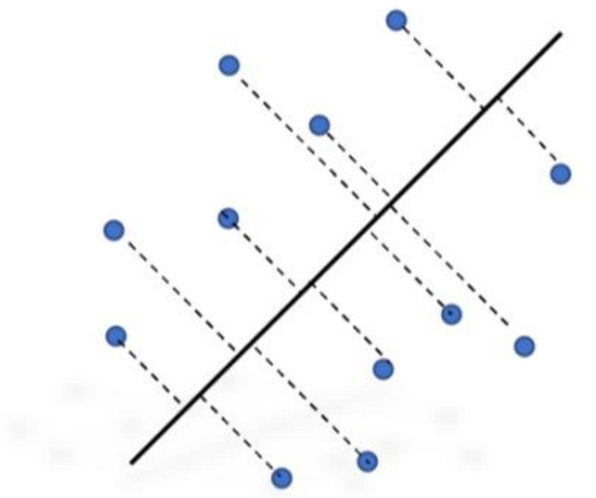
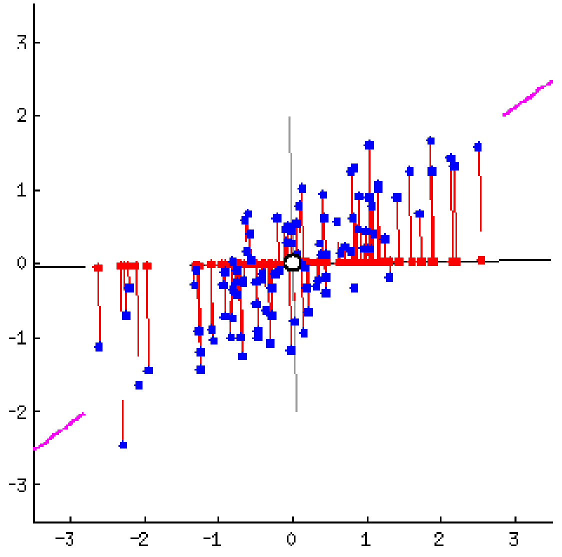


Figure 9.7: PCA: (a) the original data; (b) two principal components displayed as vectors; (c) the data projected on the first principal component. Source: The hundred-page machine learning book

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)





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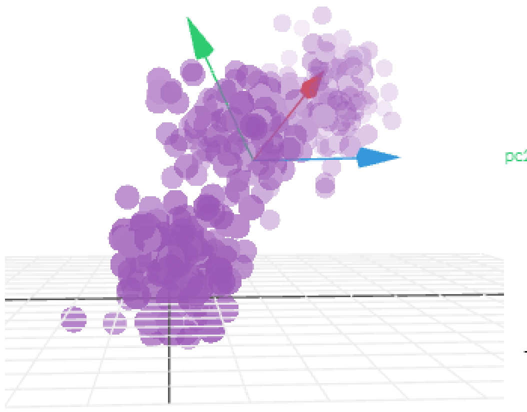
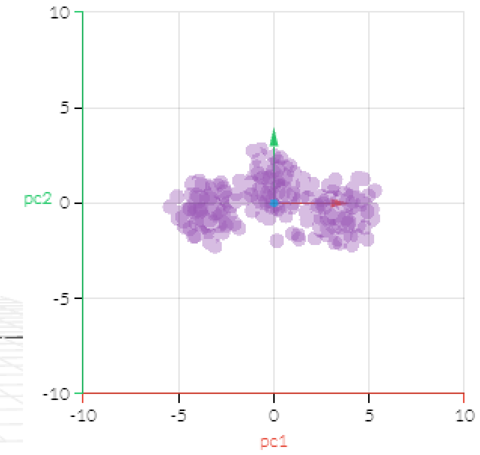
Part II

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 $X_1, X_2, \ldots, X_p$ is the normalized linear combination of the features that has the largest variance.

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

- The elements $\phi_{11}, \ldots, \phi_{p1}$ are referred to as loadings of PC1.
- Note that the X features are standardized (why?)
- The loading vector ϕ_1 defines a direction in feature space along which the data vary the most i.e., maximizing the variance in that direction!

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

USA arrests data: Biplot

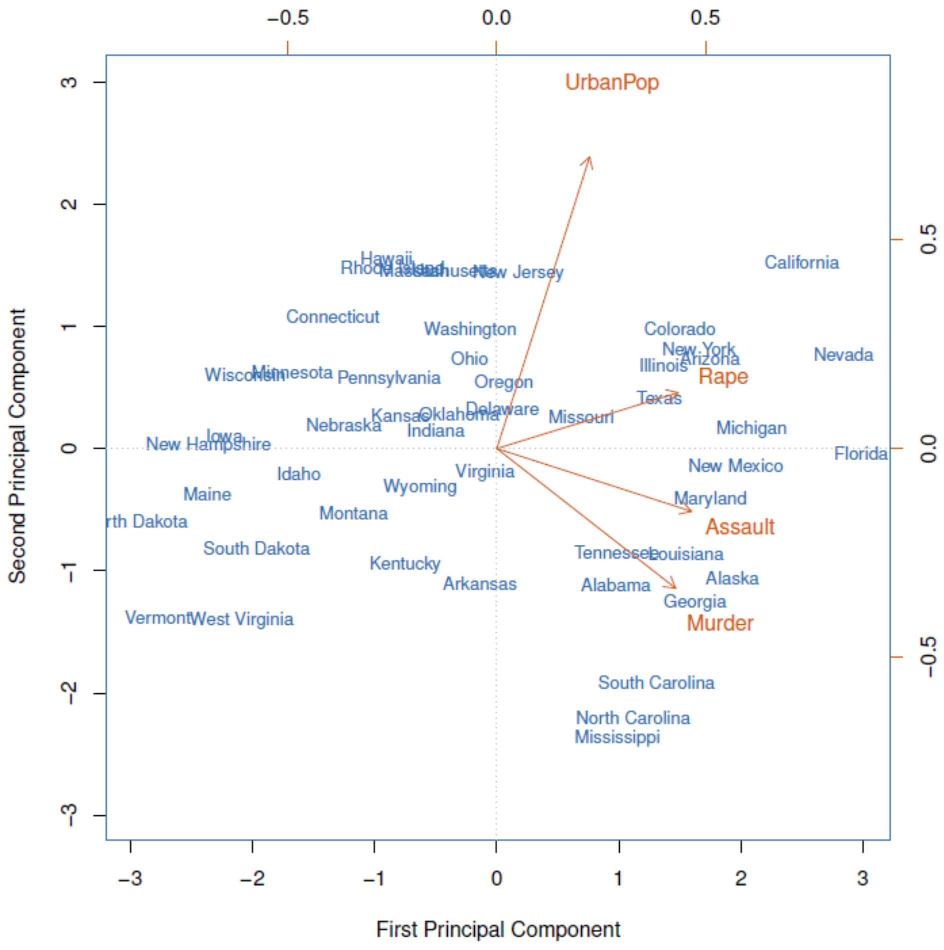
- USA arrests data contains the number of arrests per 100k residents for each of the 50 states.
- The features are murder, assault, rape and urban population.
- PCA was performed after standardizing each feature! The loadings are as follow:

	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.

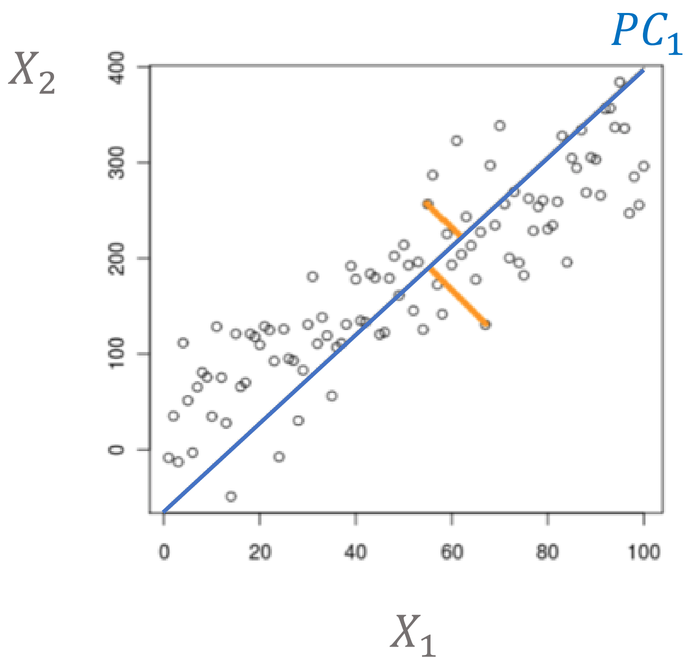
Source: ISLR first edition

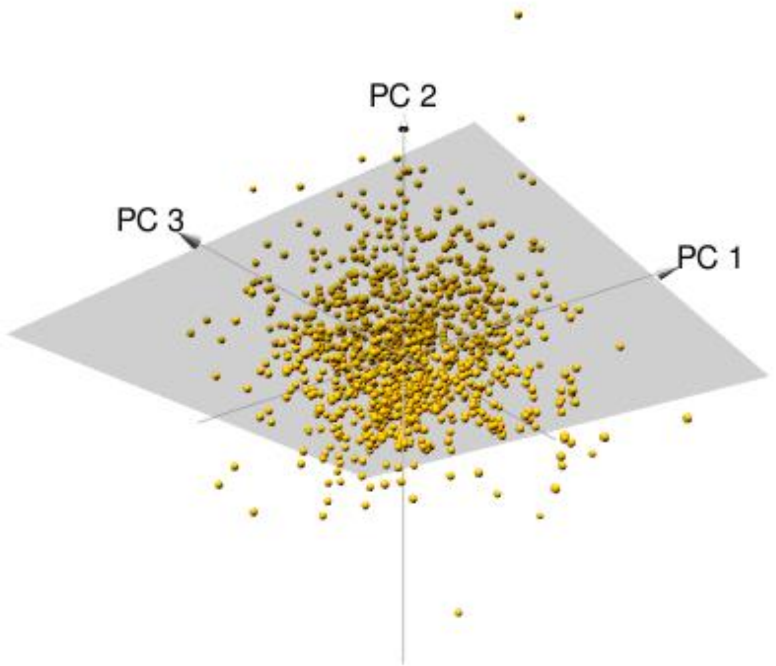
	Murder	Assault	UrbanPop	Rape
California	0.2782682	1.262814	1.7589234	2.067820
Florida	1.7476714	1.970778	0.9989801	1.138967
New Hampshire	-1.3059321	-1.365049	-0.6590781	-1.252564



Another interpretation of PCA

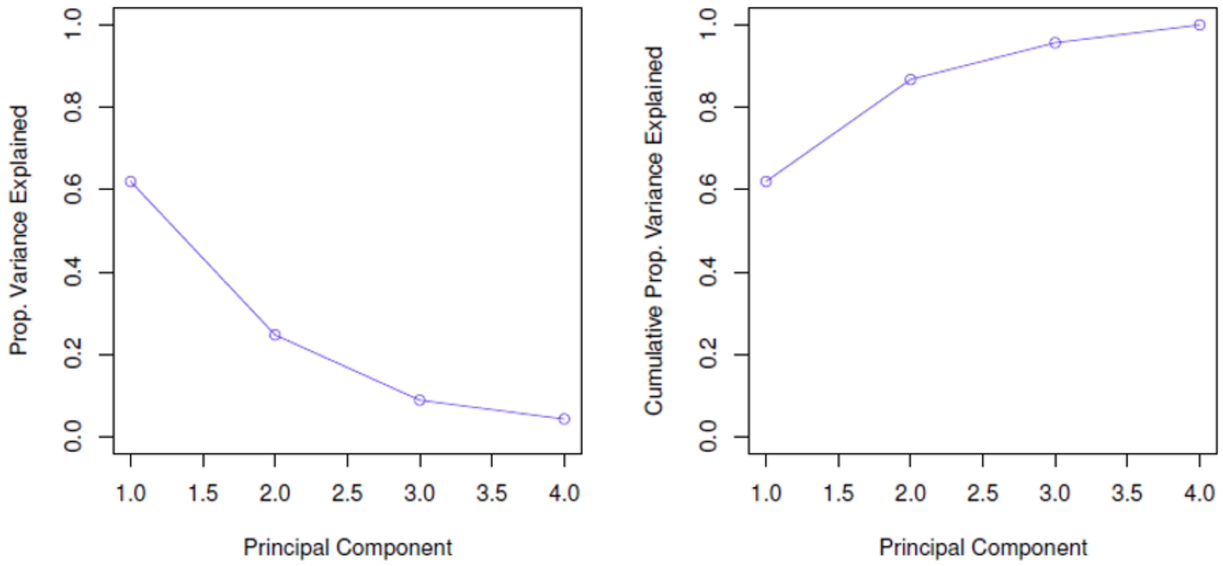
- PCA find the hyperplane closest to the observations!
- What is the difference between PCA and linear regression then?





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? Why cannot we use cross validation?

Part III

Why PCA? Pros and cons!

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 interpret if provided with lower-dimensional datasets.

Cons:

- Hard to interpret!

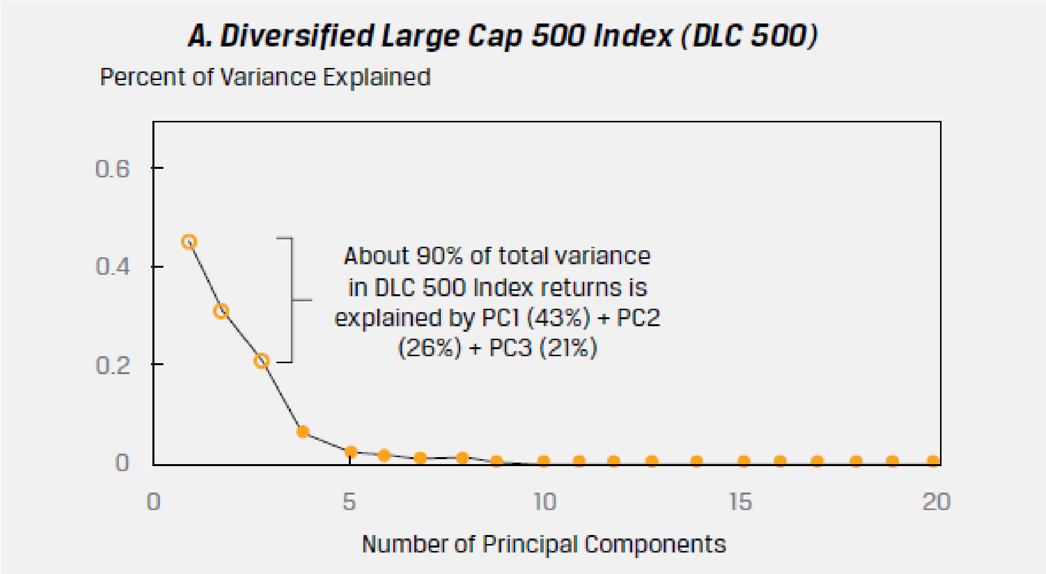
Applications of PCA (Example from CFA II reading 7)

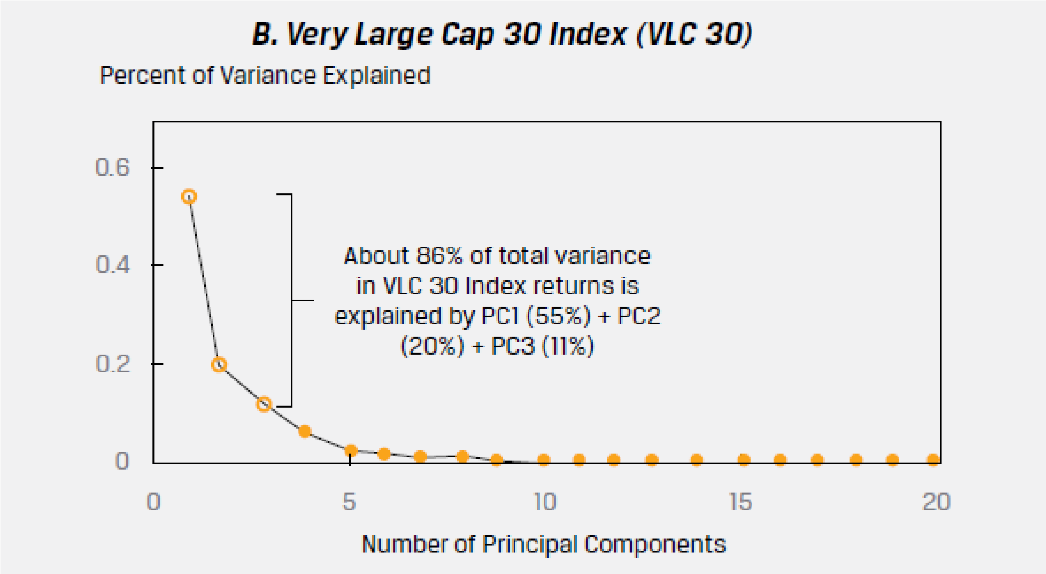
- Consider a hypothetical Diversified Large Cap (**DLC**) 500 and Very Large Cap (**VLC**) 30:
  - DLC 500 can be thought of as a diversified index of **500 large-cap companies** covering all economic sectors
  - VLC 30 is a more concentrated index of the **30 largest publicly traded companies**.

- 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 (Example from CFA II reading 7)

- 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:**