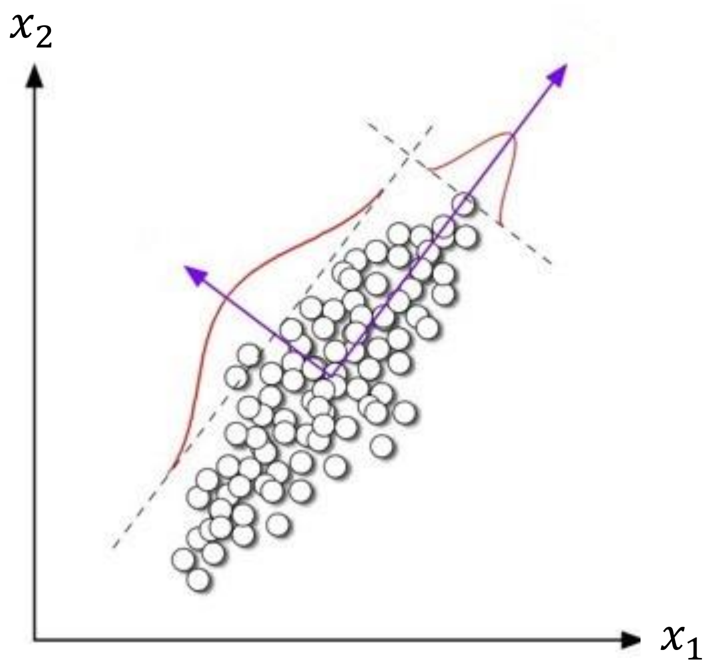
Module 11
Principal Component Analysis (PCA)

Prof. Pedram Jahangiry



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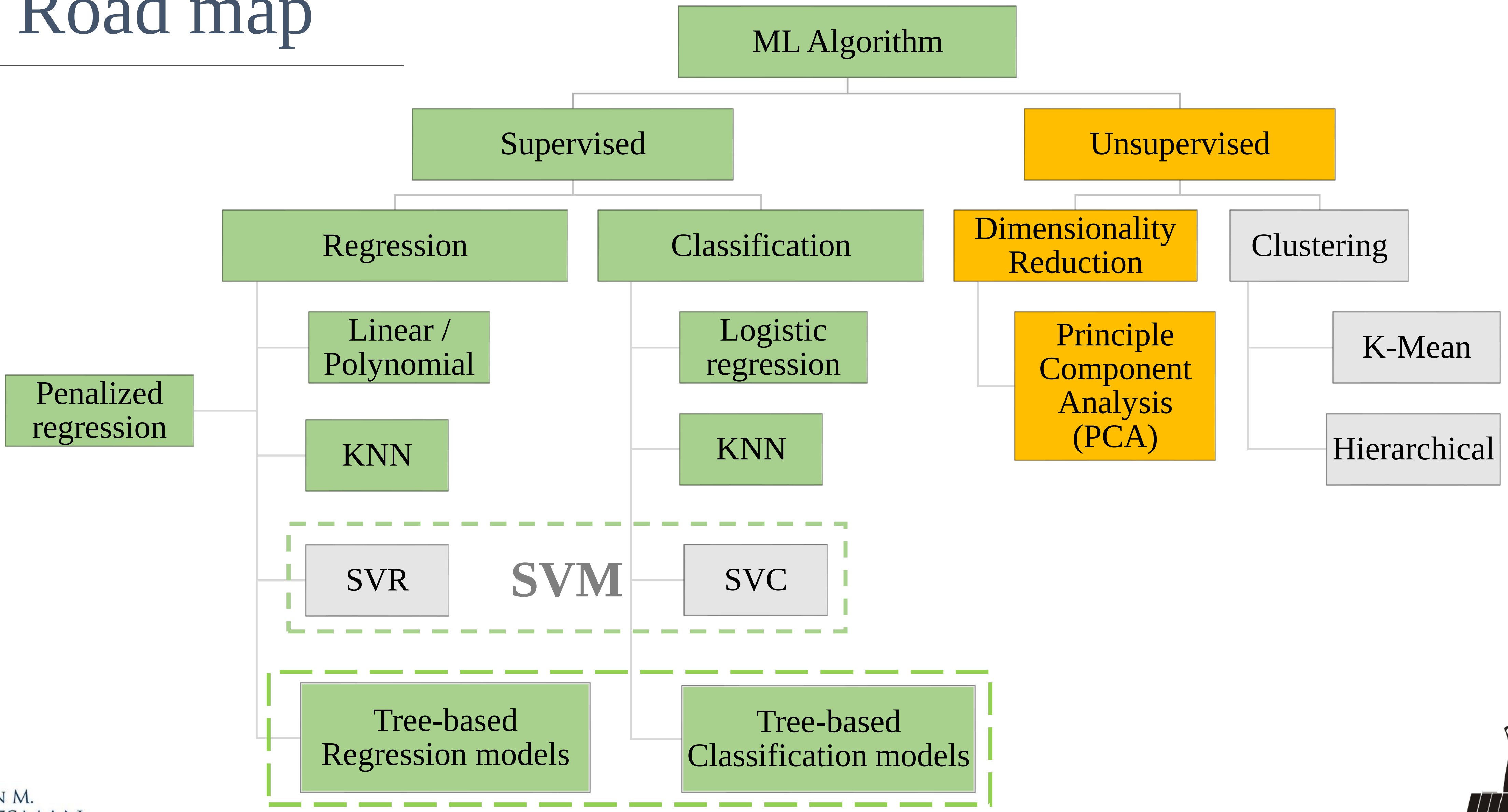
Road map



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Topics

Part I

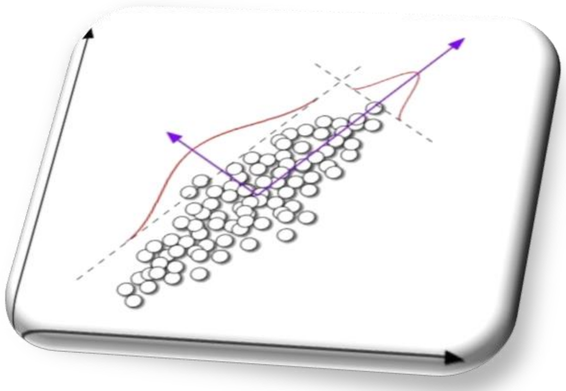
1. Unsupervised Machine Learning
2. Principal Component terminology

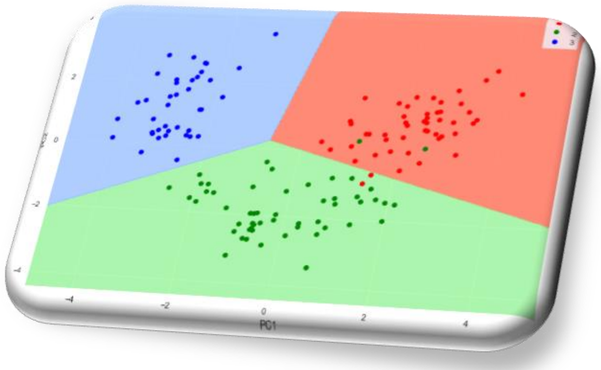
Part II

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

Part III

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





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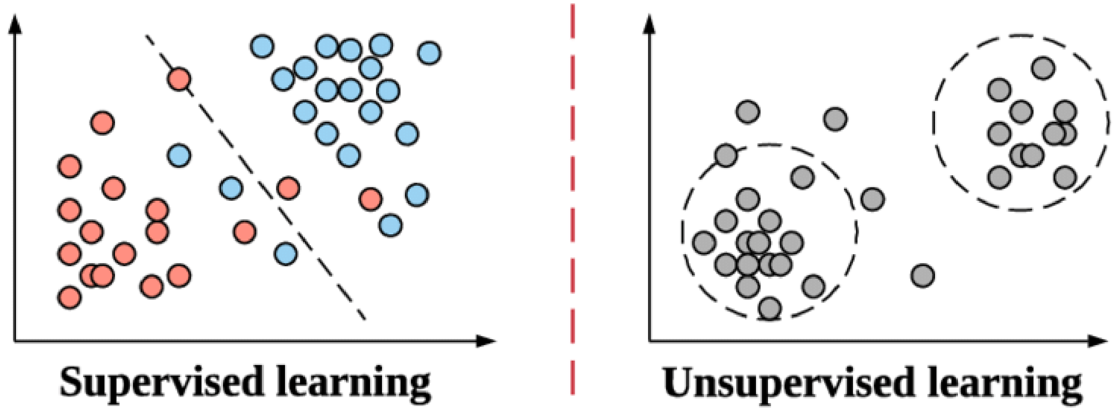
Part I

1. Unsupervised Machine Learning
2. PC terminology

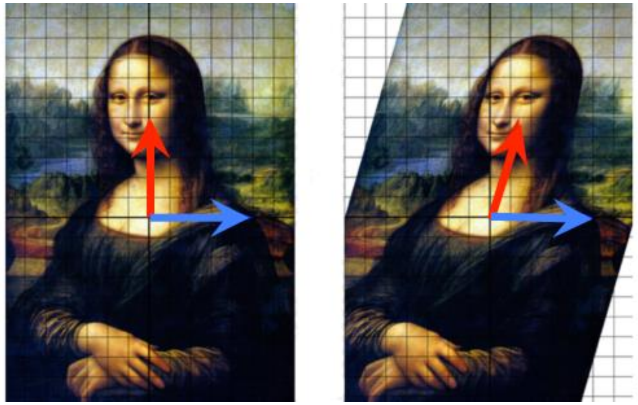
Unsupervised Learning

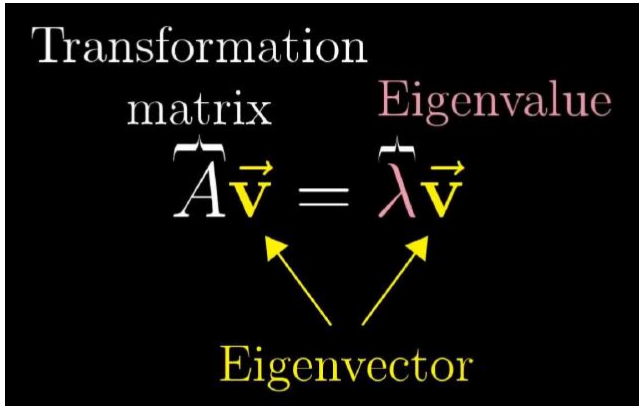
- Unsupervised learning is a machine learning technique that does not use labeled data (no target variable)
- The goal is to discover the underlying patterns and find groups of samples that behave similarly.
- The two main types of unsupervised learning algorithms are:
  1) Dimension reduction algorithm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

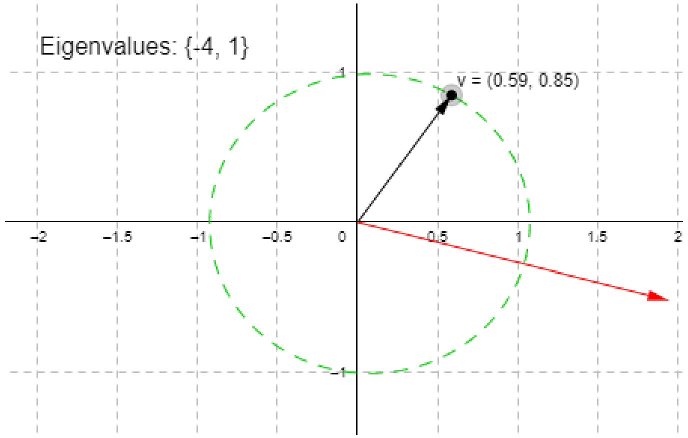


Eigen things!

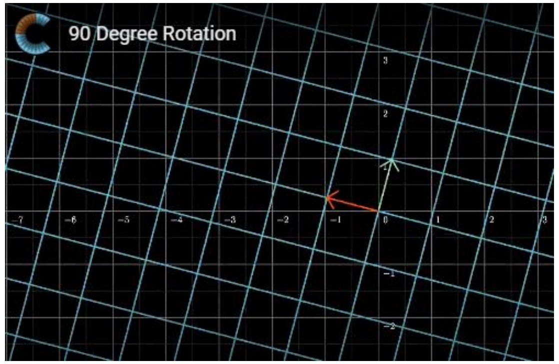
- Eigenvector does not change direction in a transformation.
- In this mapping, the blue arrow is eigenvector (why?)
- Its eigenvalue = 1 (why?)
- For a square matrix A, an Eigenvector and Eigenvalue are defined as follow:





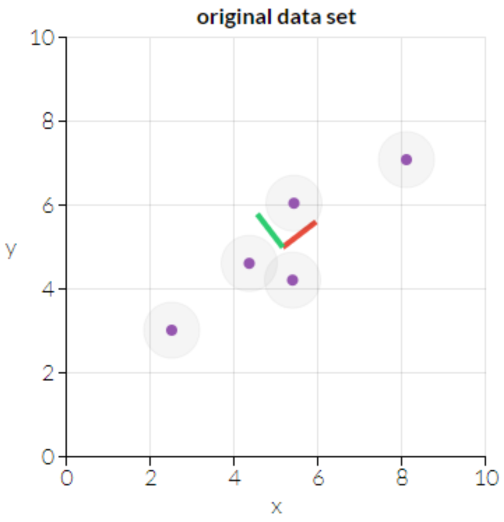


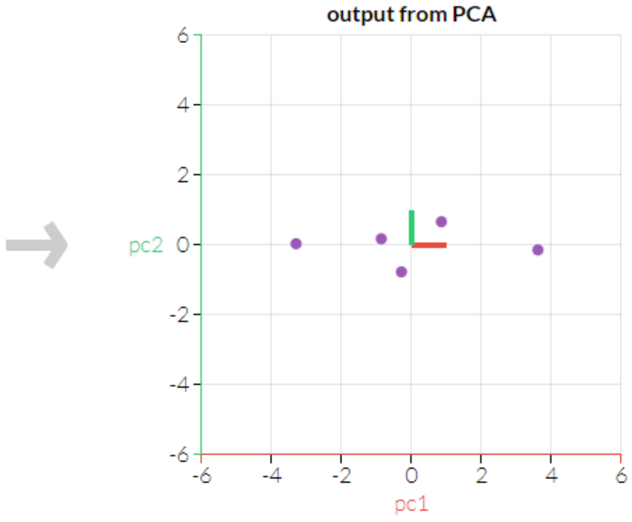
What is a transformation matrix?



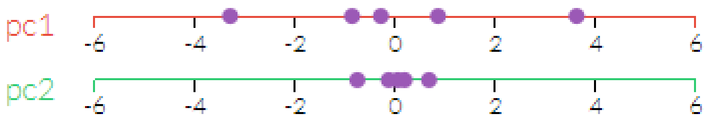
PC terminology (connecting PC and Eigenthings)

- 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**.

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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.

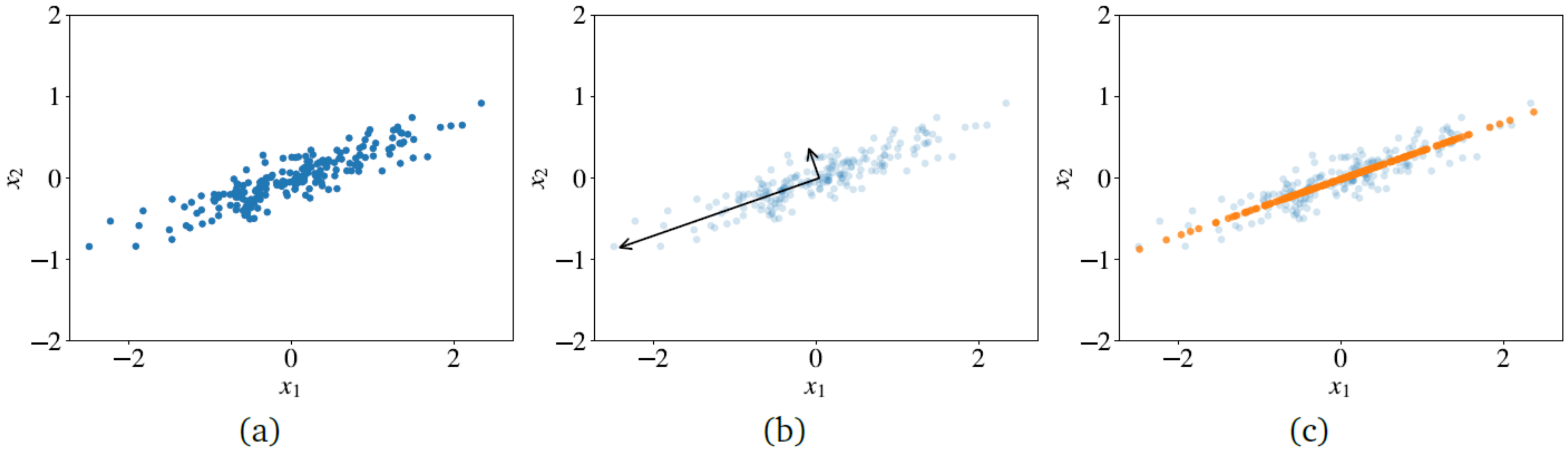
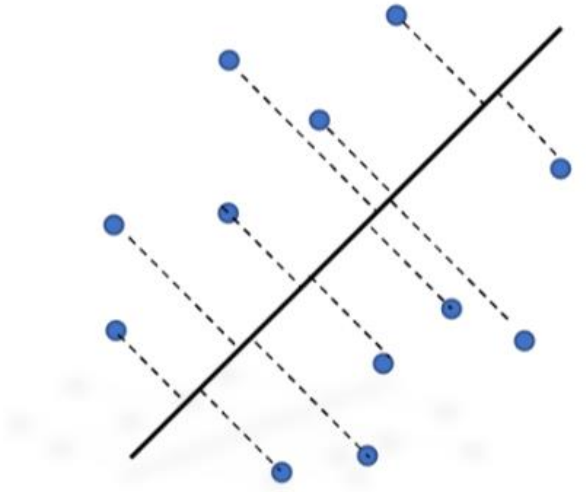
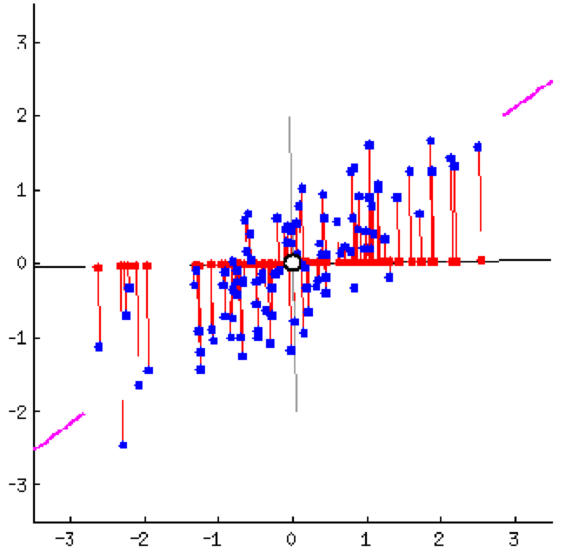


Figure 9.7: PCA: (a) the original data; (b) two principal components displayed as vectors; (c) the data projected on the first principal component. Source: The hundred-page machine learning book

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)



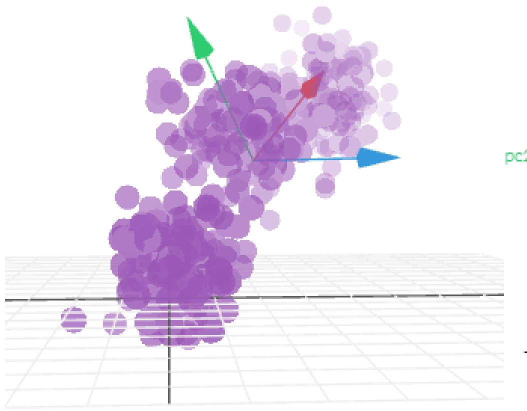


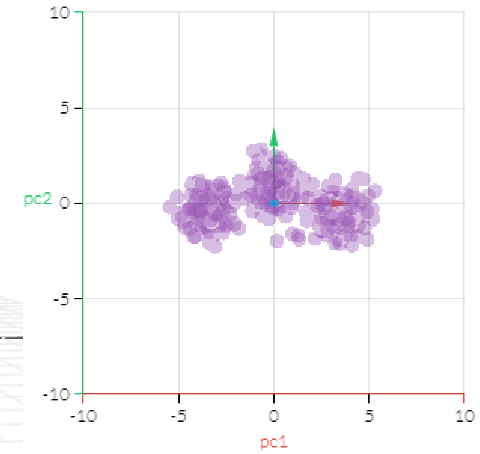
Part II

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 ϕ_1 defines a direction in feature space along which the data vary the most i.e., maximizing the variance in that direction!

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

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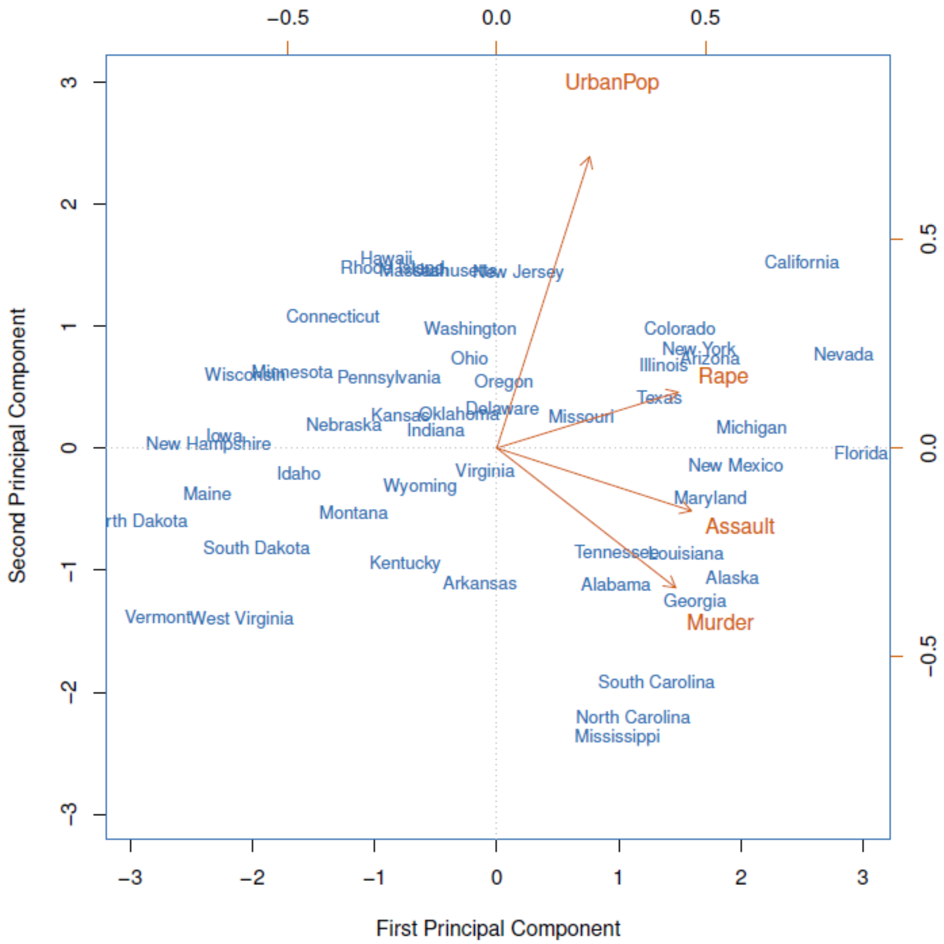
USA arrests data: Biplot

- 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:

```
              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
```

	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

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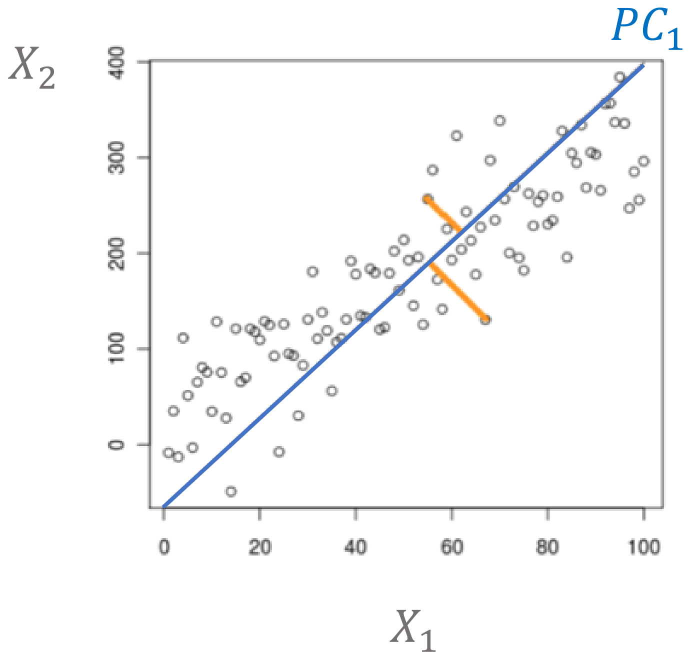
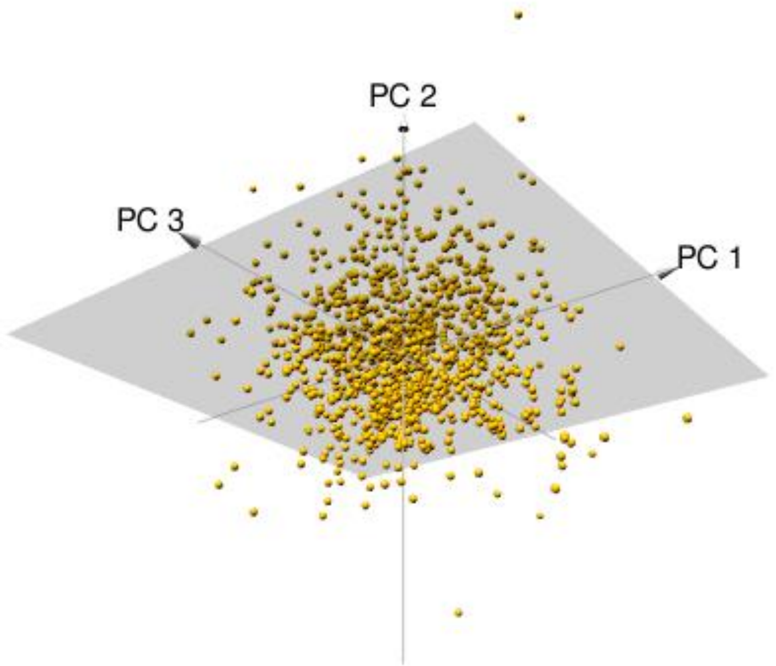
Another interpretation of PCA

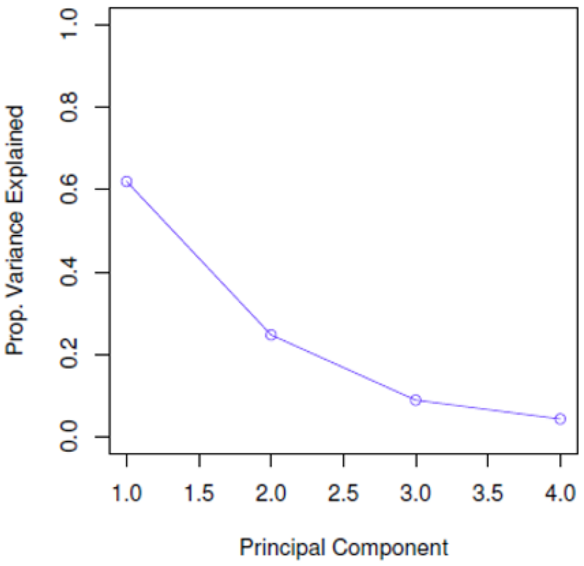
- PCA find the hyperplane closest to the observations!
- What is the difference between PCA and linear regression then?

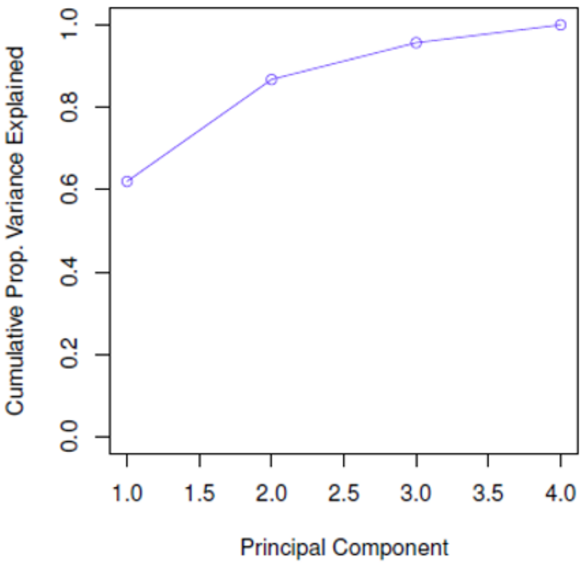




Scree plot

- 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? 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!

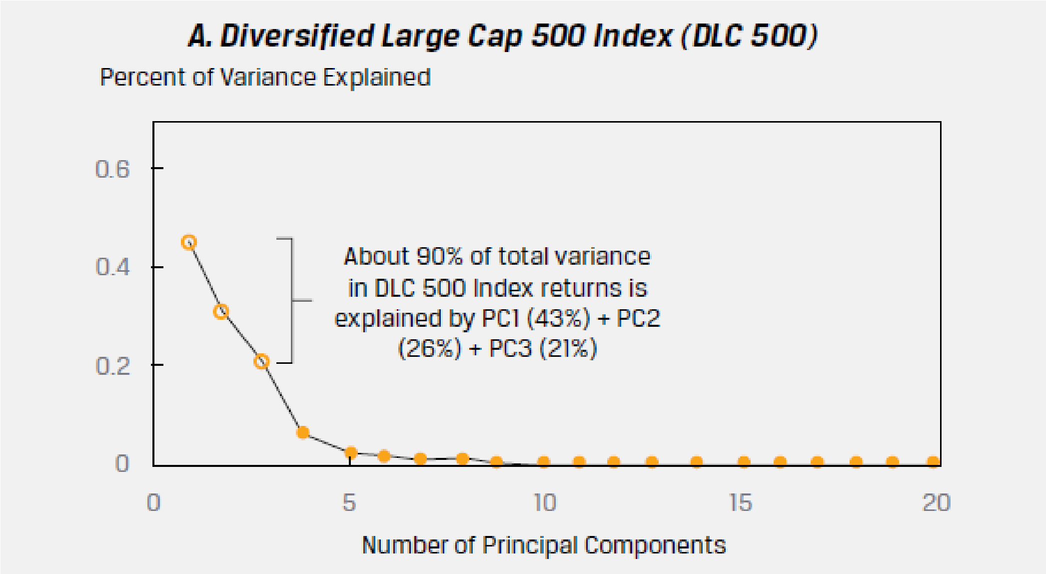
Applications of PCA (Example from CFA II reading 7)

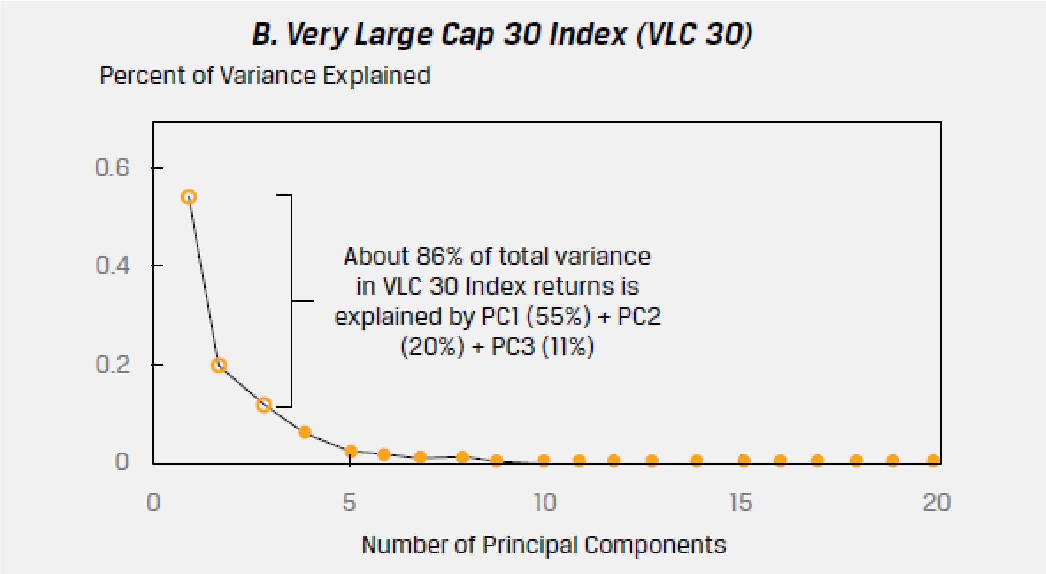
- Consider a hypothetical Diversified Large Cap (**DLC**) 500 and Very Large Cap (**VLC**) 30:
  - DLC 500 can be thought of as a diversified index of **500 large-cap companies** covering all economic sectors
  - VLC 30 is a more concentrated index of the **30 largest publicly traded companies**.

- 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)

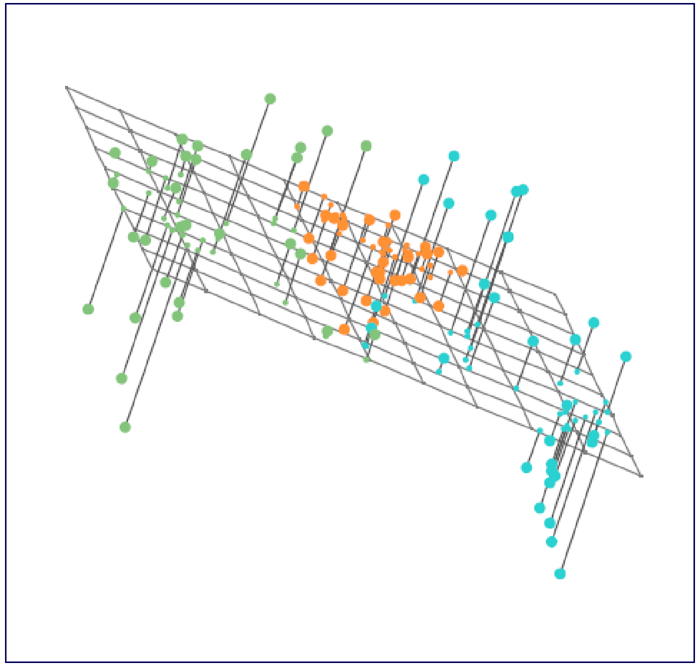
- The following scree plots show that of the 20 principal components generated, **the first 3 together** explain about 90% of the variance of DLC 500 and 86% of the VLC 30.

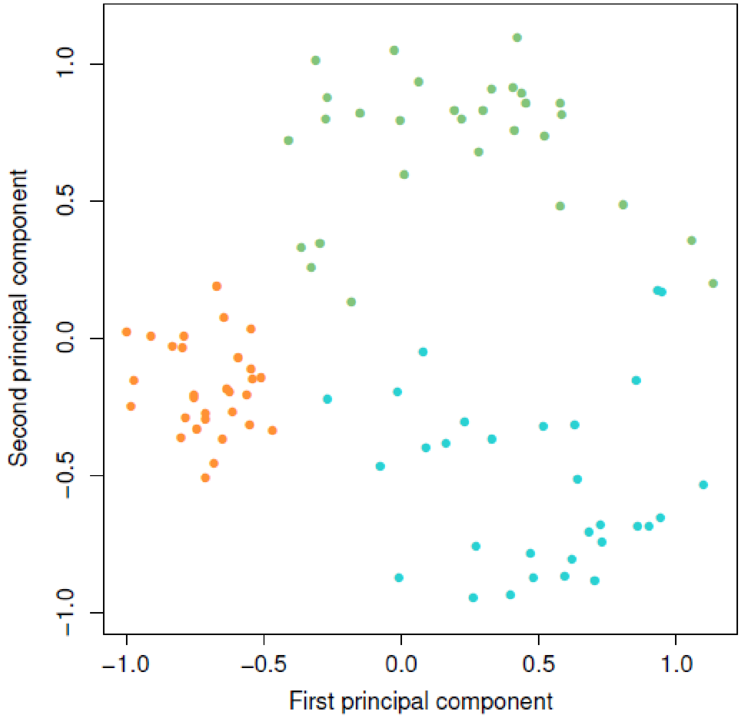




Applications of PCA (Data visualization)

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





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. It is like the idea of Support Vector Machines.
- Using PCA with a supervised learning model like logistic regression: