ĐẠI HỌC BÁCH KHOA

25 YEARS ANNIVERSARY SOICT

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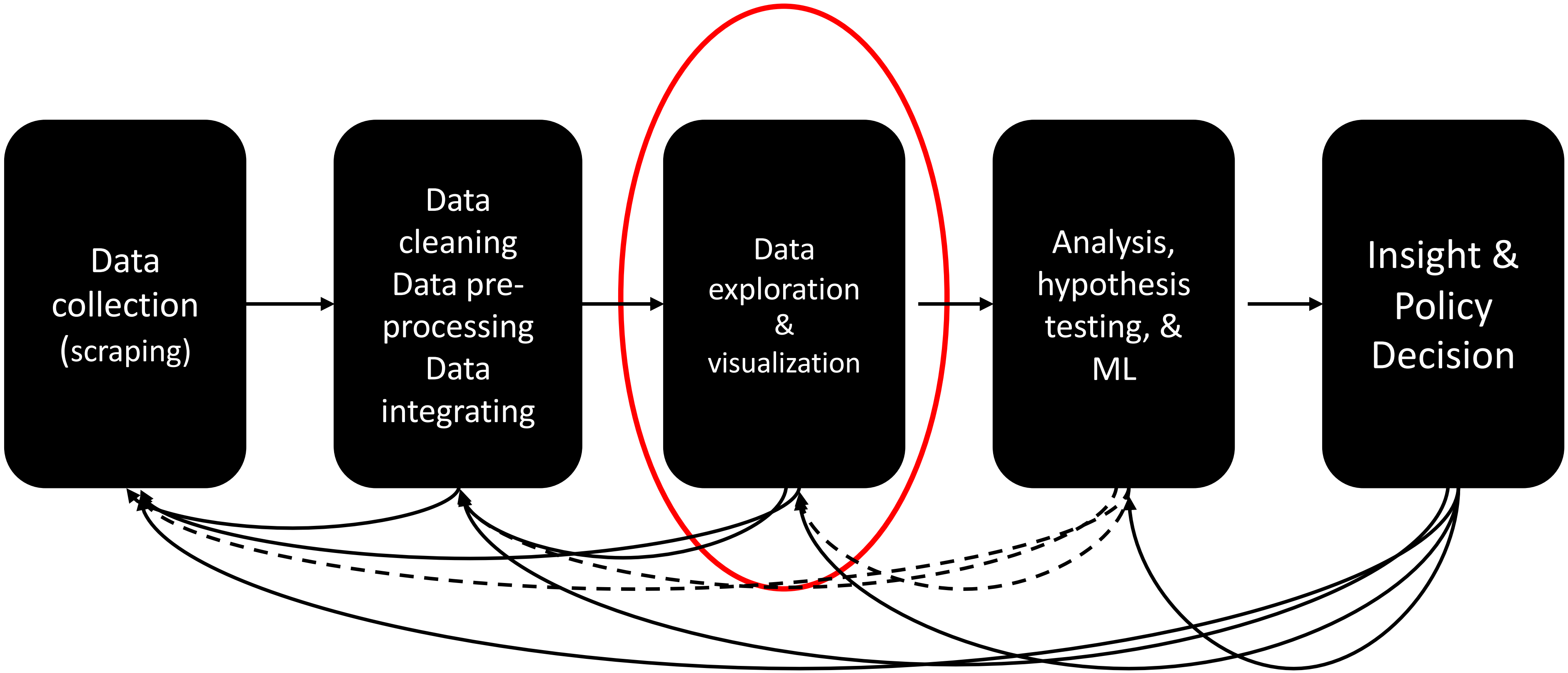
Lecture 5
Exploratory Data Analysis
(EDA)

Learning outcomes

- Understand key elements in exploratory data analysis (EDA)
- Explain and use common summary statistics for EDA
- Plot and explain common graphs and charts for EDA

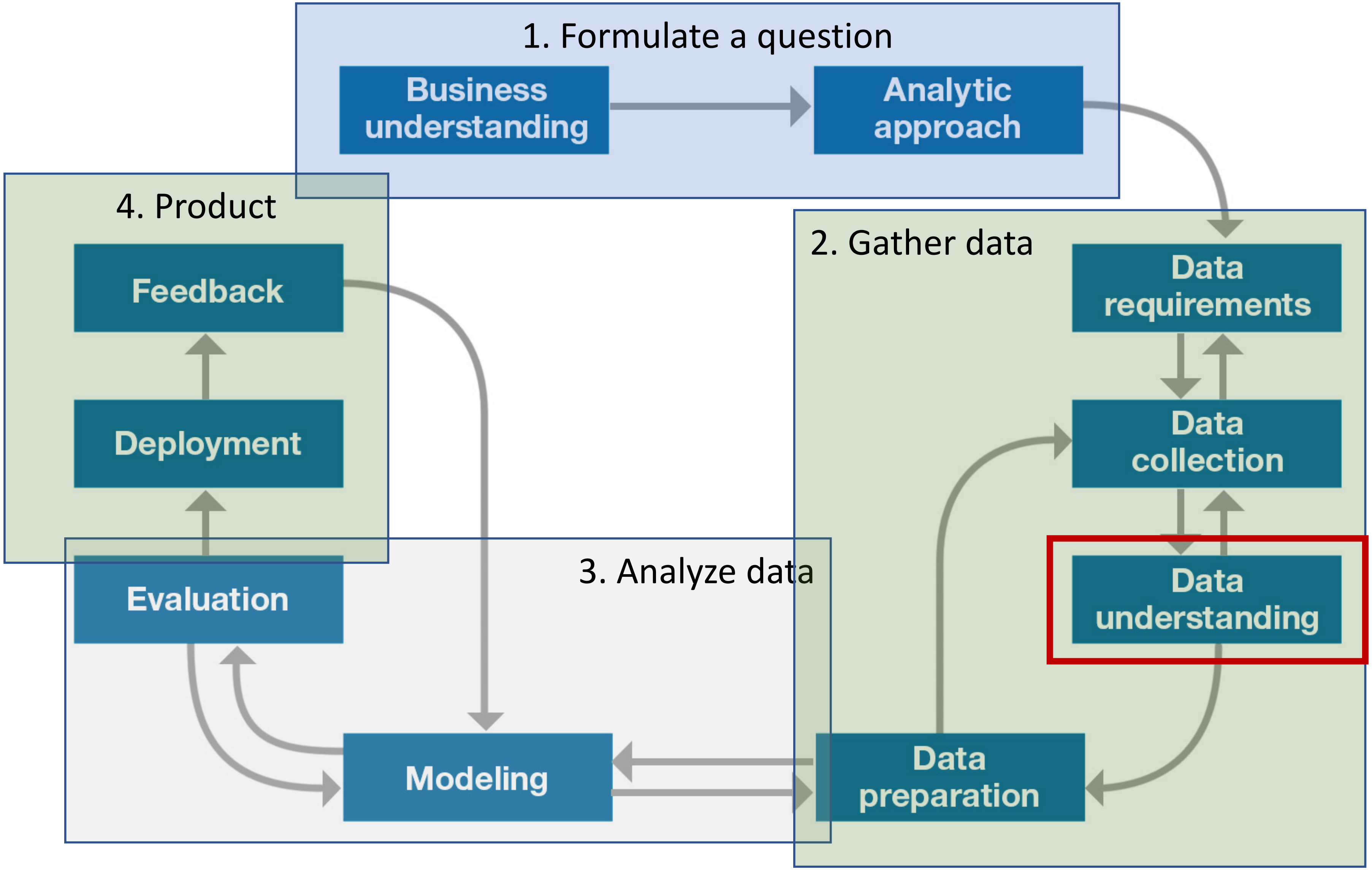
Recall: insight-driven DS methodology



Motivation

- Before making inferences from data it is essential to examine all your variables.
    - To understand your data
- Why?
    - To listen to the data:
    - to catch mistakes
    - to see patterns in the data
    - to find violations of statistical assumptions
    - to generate hypotheses
    - …and because if you don’t, you will have trouble later

Data science process



Source: *Foundational Methodology for Data Science*, IBM, 2015

Exploratory data analysis (EDA) focus

- The focus is on the data—its structure, outliers, and models suggested by the data.
- EDA approach makes use of (and shows) all of the available data. In this sense there is no corresponding loss of information.
    - Summary statistics
    - Visualization
    - Clustering and anomaly detection
    - Dimensionality reduction

EDA definition

- The EDA is precisely not a set of techniques, but an attitude/philosophy about how a data analysis should be carried out.
  - Helps to select the right tool for preprocessing or analysis
  - Makes use of humans' abilities to recognize patterns in data

EDA common questions

- What is a typical value?
- What is the uncertainty for a typical value?
- What is a good distributional fit for a set of numbers?
- Does an engineering modification have an effect?
- Does a factor have an effect?
- What are the most important factors?
- Are measurements coming from different laboratories equivalent?
- What is the best function for relating a response variable to a set of factor variables?
- What are the best settings for factors?
- Can we separate signal from noise in time dependent data?
- Can we extract any structure from multivariate data?
- Does the data have outliers?

EDA is an iterative process

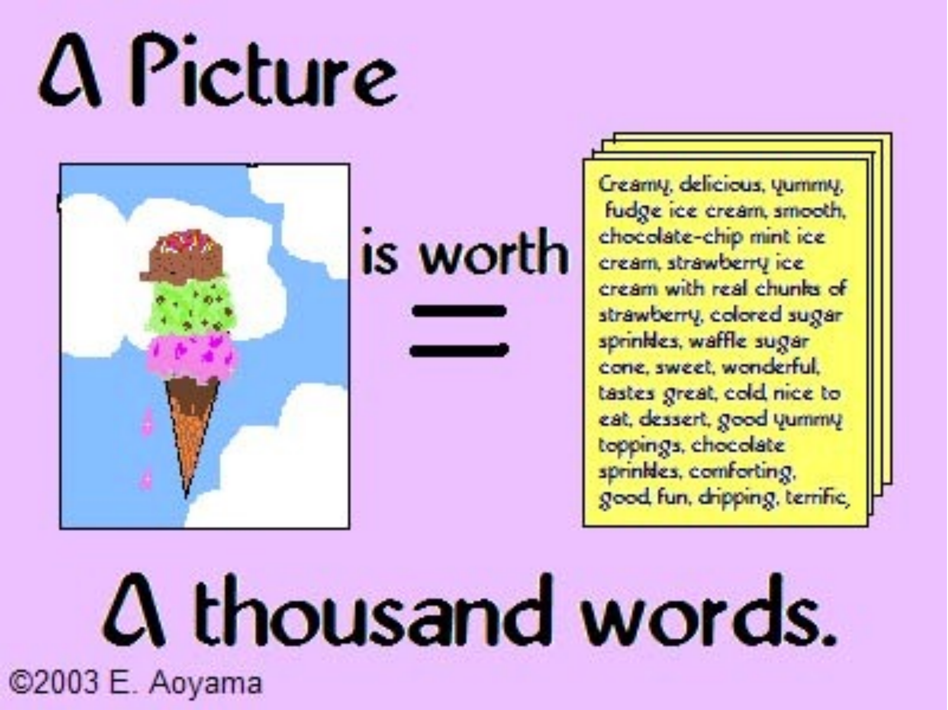
- **Repeat...**
  - Identify and prioritize relevant questions in decreasing order of importance
  - Ask questions
  - Construct graphics to address questions
  - Inspect “answer” and derive new questions

EDA strategy

- Examine variables one by one, then look at the relationships among the different variables
- Start with graphs, then add numerical summaries of specific aspects of the data
- Be aware of attribute types
  - Categorical vs. Numeric

EDA techniques

- Graphical techniques
  - scatter plots, character plots, box plots, histograms, probability plots, residual plots, and mean plots.
- Quantitative techniques



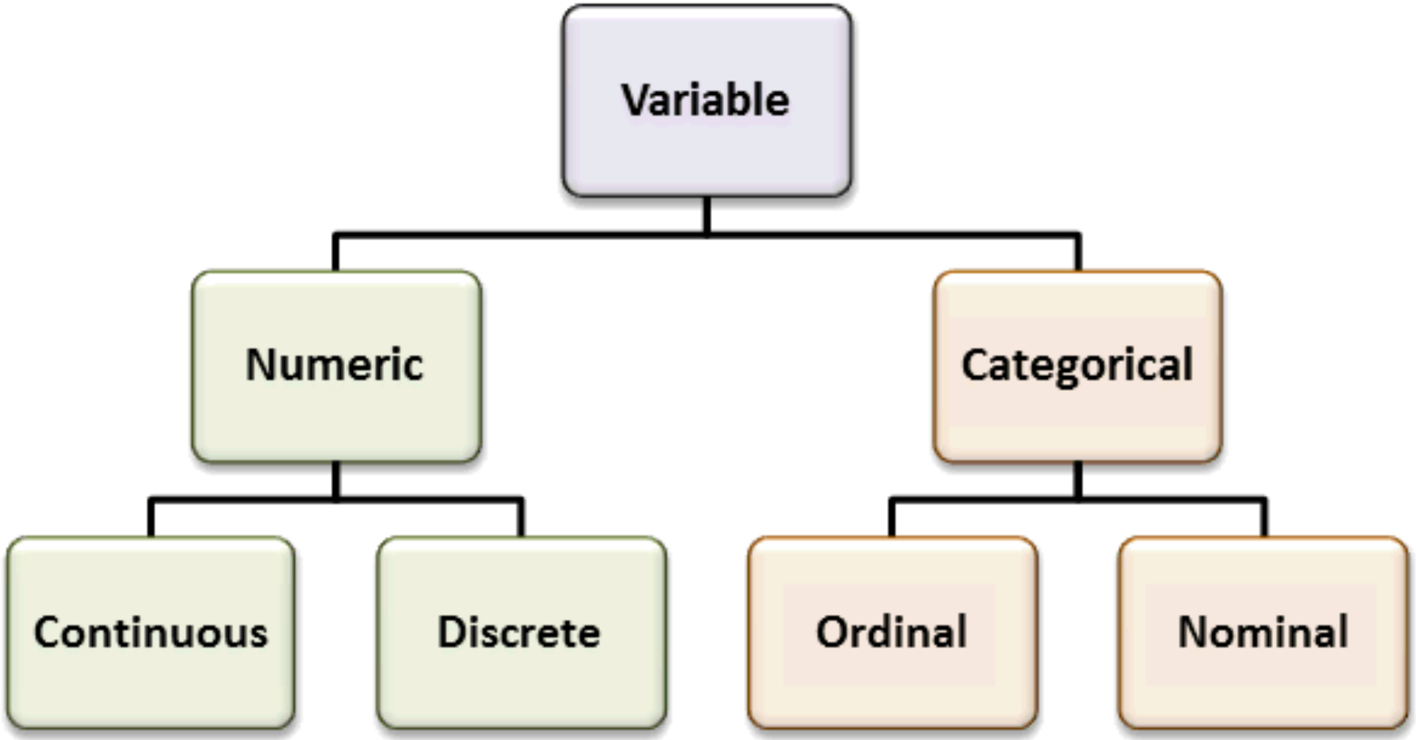
Describing univariate data

Observations and variables

- Data is an collection of observations
- an attribute is thought of as a set of values describing some aspect across all observations, it is called a variable

HR Information		Contact	
Position	**Salary**	**Office**	**Extn.**
Accountant	$162,700	Tokyo	5407
Chief Executive Officer (CEO)	$1,200,000	London	5797
Junior Technical Author	$86,000	San Francisco	1562
Software Engineer	$132,000	London	2558

Types of variables



Dimensionality of data sets

- Univariate: Measurement made on one variable per subject
- Bivariate: Measurement made on two variables per subject
- Multivariate: Measurement made on many variables per subject

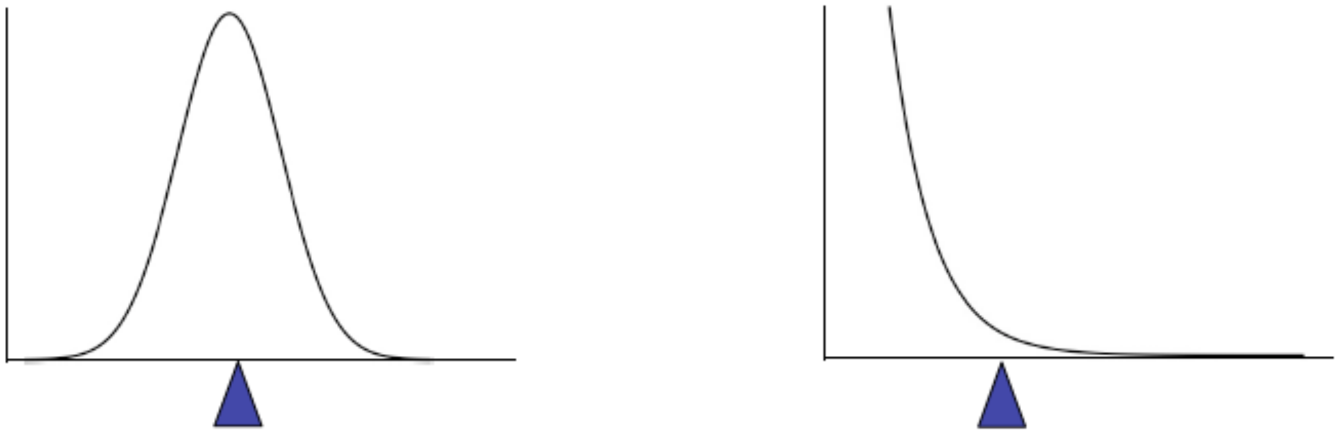
Measures of central tendency

- Measures of Location: estimate a location parameter for the distribution; i.e., to find a typical or central value that best describes the data.
- Measures of Scale: characterize the spread, or variability, of a data set. Measures of scale are simply attempts to estimate this variability.
- Skewness and Kurtosis

Mean

- To calculate the average value of a set of observations, sum of their values divided by the number of observations:

$$\bar{x} = \frac{x_1 + x_2 + x_3 + \ldots + x_n}{n} = \frac{1}{n}\sum_{i=1}^{n} x_i$$



Median

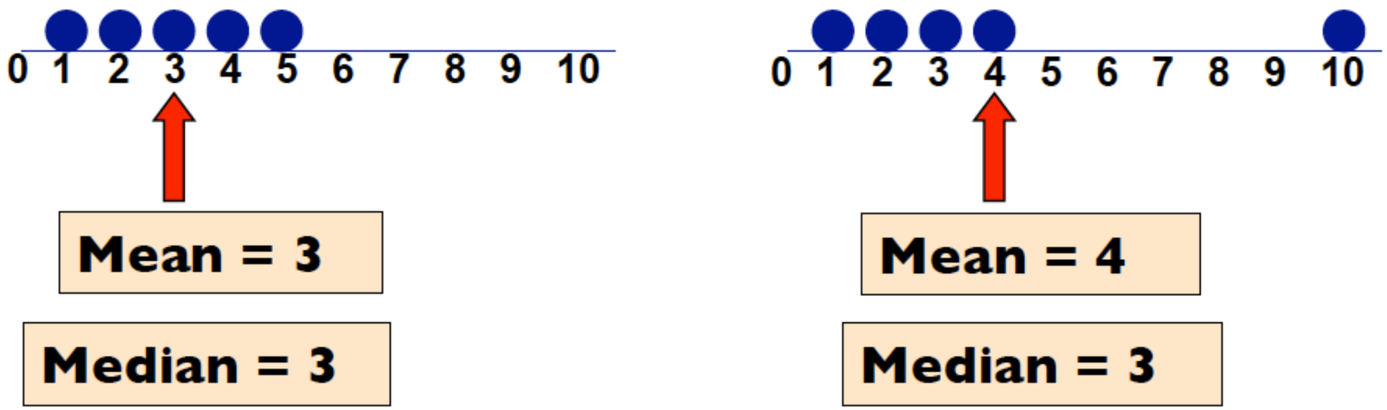
- The median is the value of the point which has half the data smaller than that point and half the data larger than that point.
- Calculation
  - If there are an odd number of observations, find the middle value
  - If there are an even number of observations, find the middle two values and average them
- Example
  - Age of participants: 17 19 21 22 23 23 23 38
  - **Median = (22+23)/2 = 22.5**

Mode

- mode is the most commonly reported value for a particular variable
  - Eg. 3, 4, 5, 6, 7, 7, 7, 8, 8, 9. Mode = 7
  - Eg. 3, 4, 5, 6, 7, 7, 7, 8, 8, 8, 9. Mode = {7, 8} = 7.5

Which location measure is best?

- Mean is best for symmetric distributions without outliers
- Median is useful for skewed distributions or data with outliers



Measure of scale : Variance and standard deviation

- Variance: average of squared deviations of values from the mean

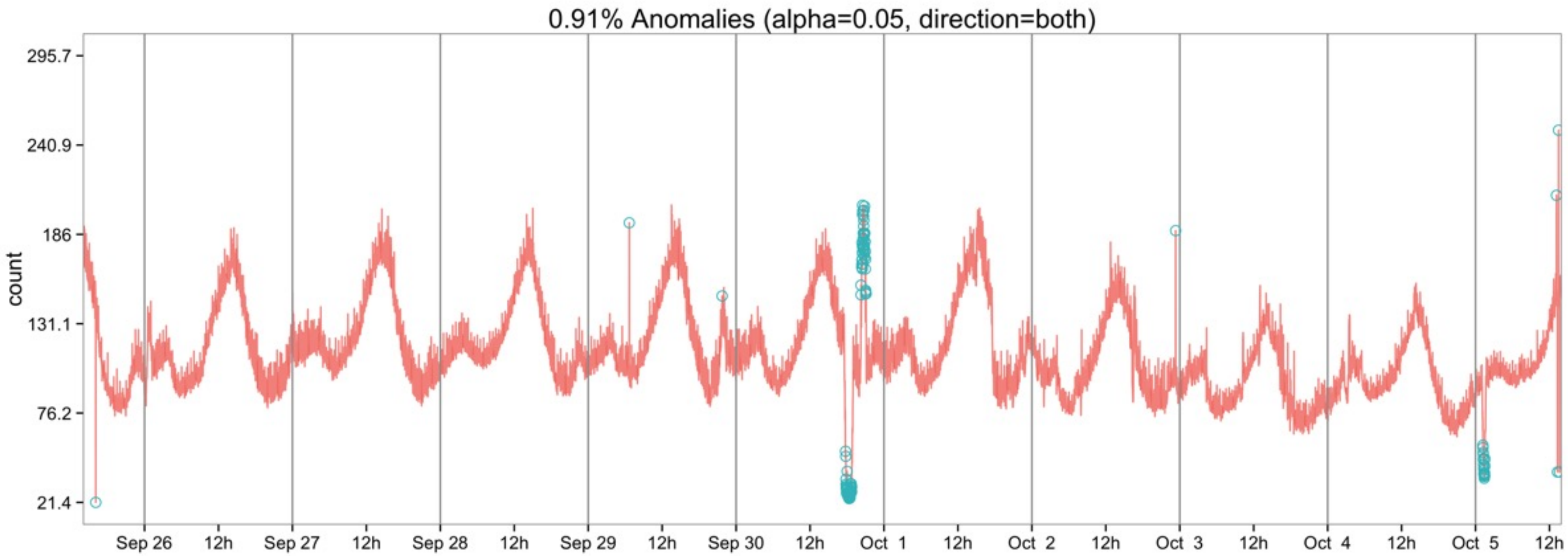
$$\hat{\sigma}^2 = \frac{\sum_{i}^{n}(x_i - \bar{x})^2}{n-1}$$

- Standard Deviation: simply the square root of the variance

$$\hat{\sigma} = \sqrt{\frac{\sum_{i}^{n}(x_i - \bar{x})^2}{n-1}}$$

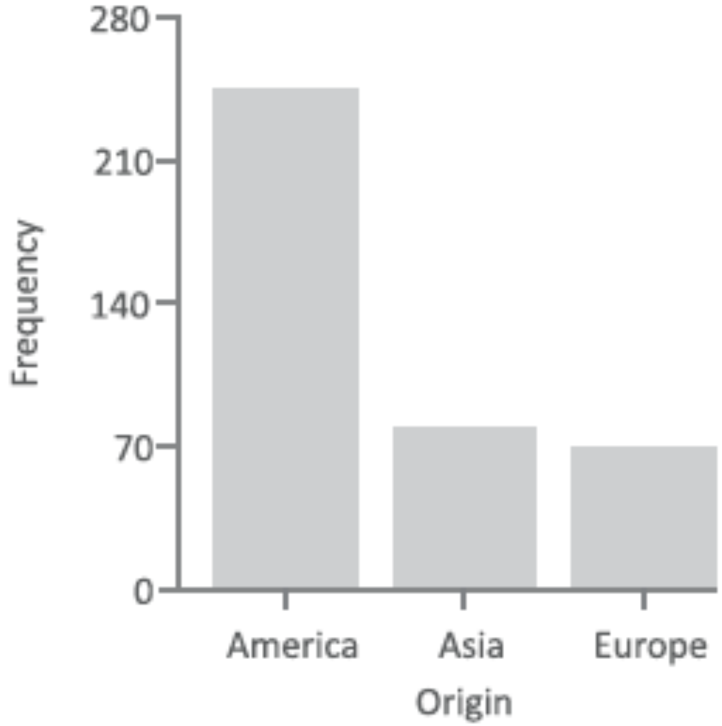
Run sequence plot

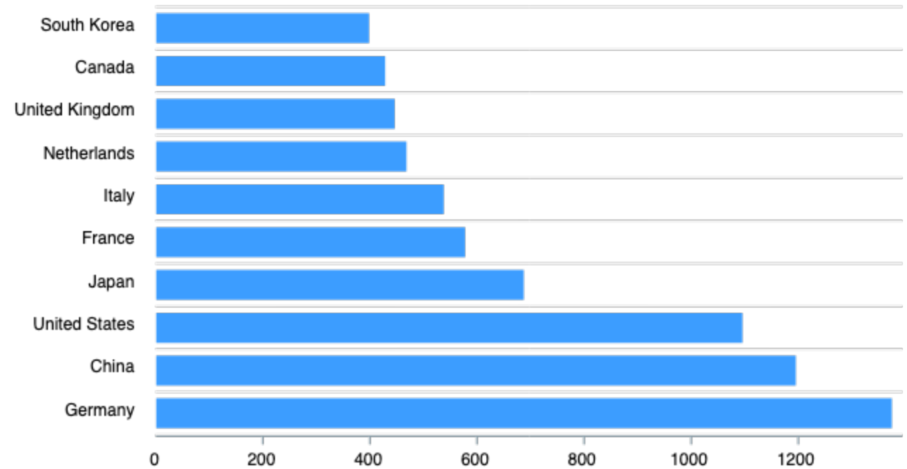
- displays observed data in a time sequence.
- The run sequence plot can be used to answer the following questions
  - Are there any shifts in location?
  - Are there any shifts in variation?
  - Are there any outliers?



Bar charts

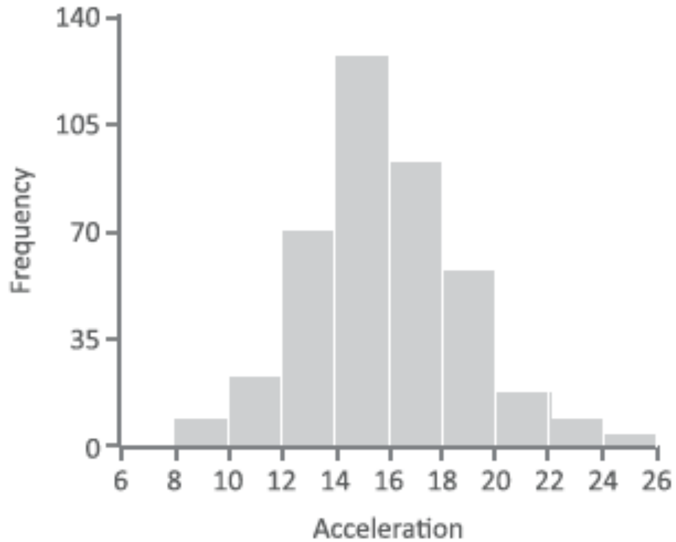
- a bar chart displays the relative frequencies for the different values.
- or a chart presents categorical data with rectangular bars with heights or lengths proportional to the values that they represent



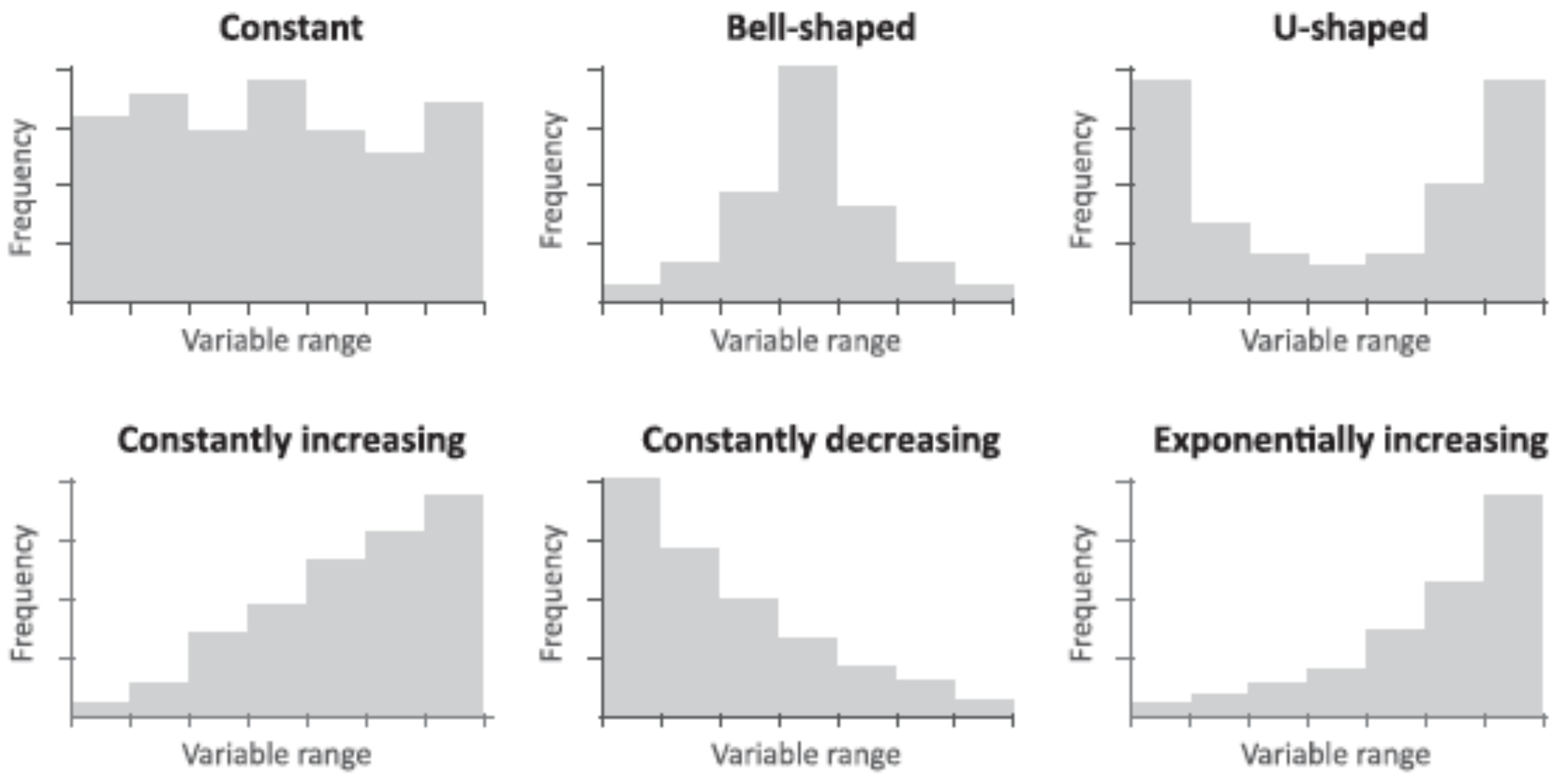


Histogram plot

- A histogram is to graphically summarize the distribution of a univariate data set.
- The histogram can be used to answer the following questions:
  - What kind of population distribution do the data come from?
  - Where are the data located?
  - How spread out are the data?
  - Are the data symmetric or skewed?
  - Are there outliers in the data?

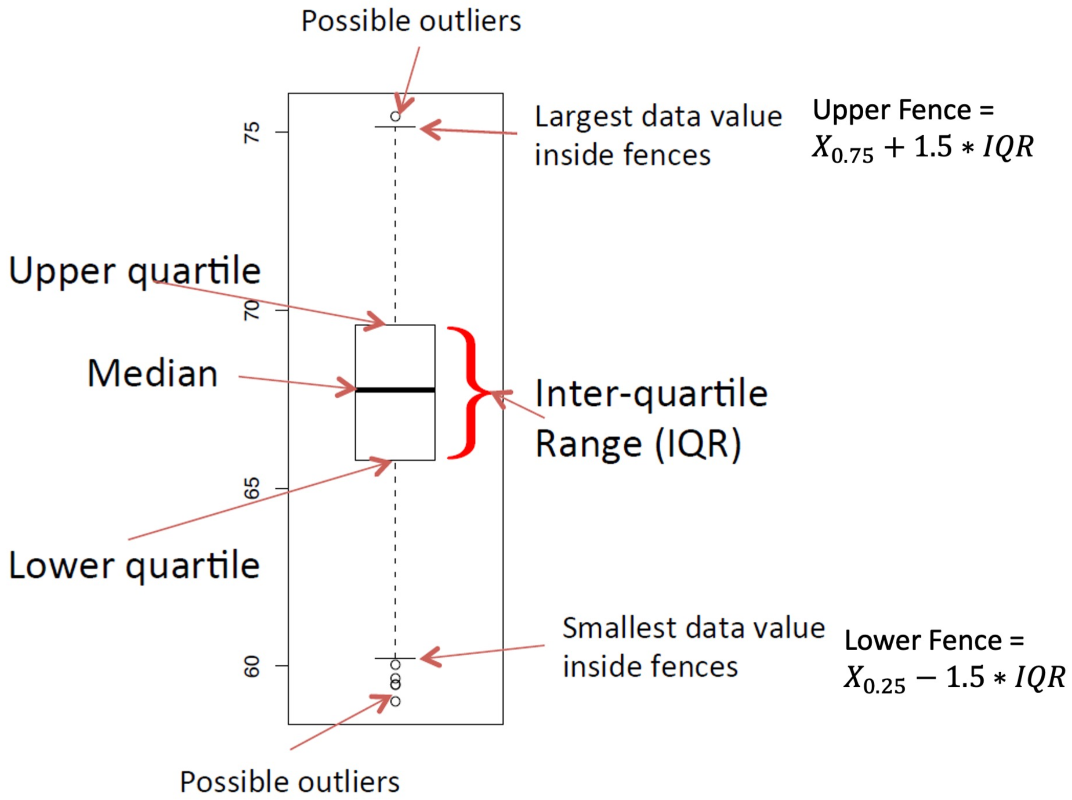


Example of frequency distributions



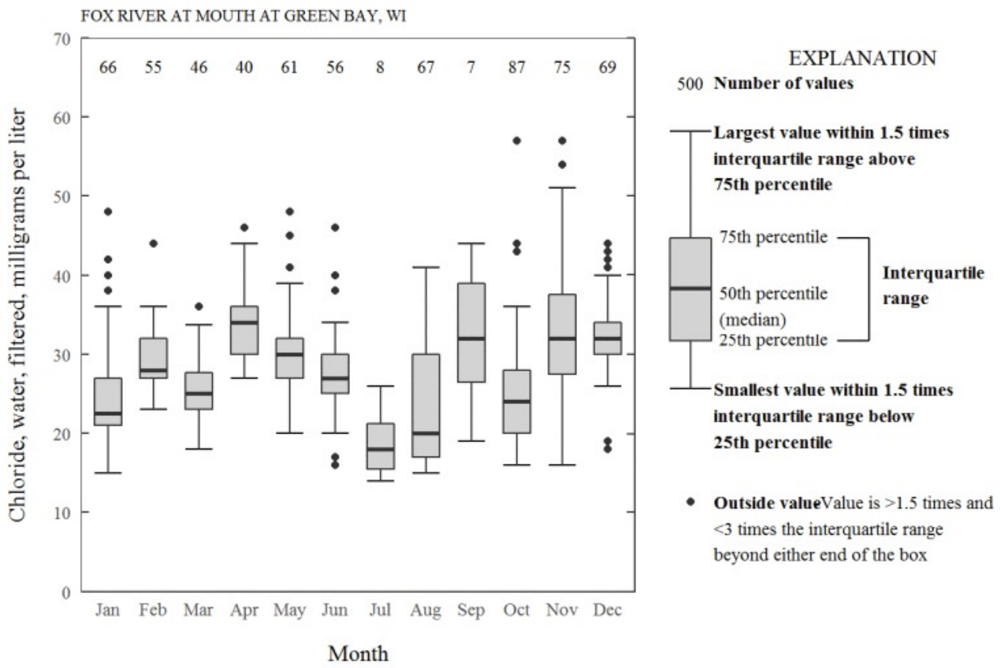
Box plot

- Box plot displayed: the lowest value, the lower quartile (Q1), the median (Q2), the upper quartile (Q3), the highest value, and the mean.



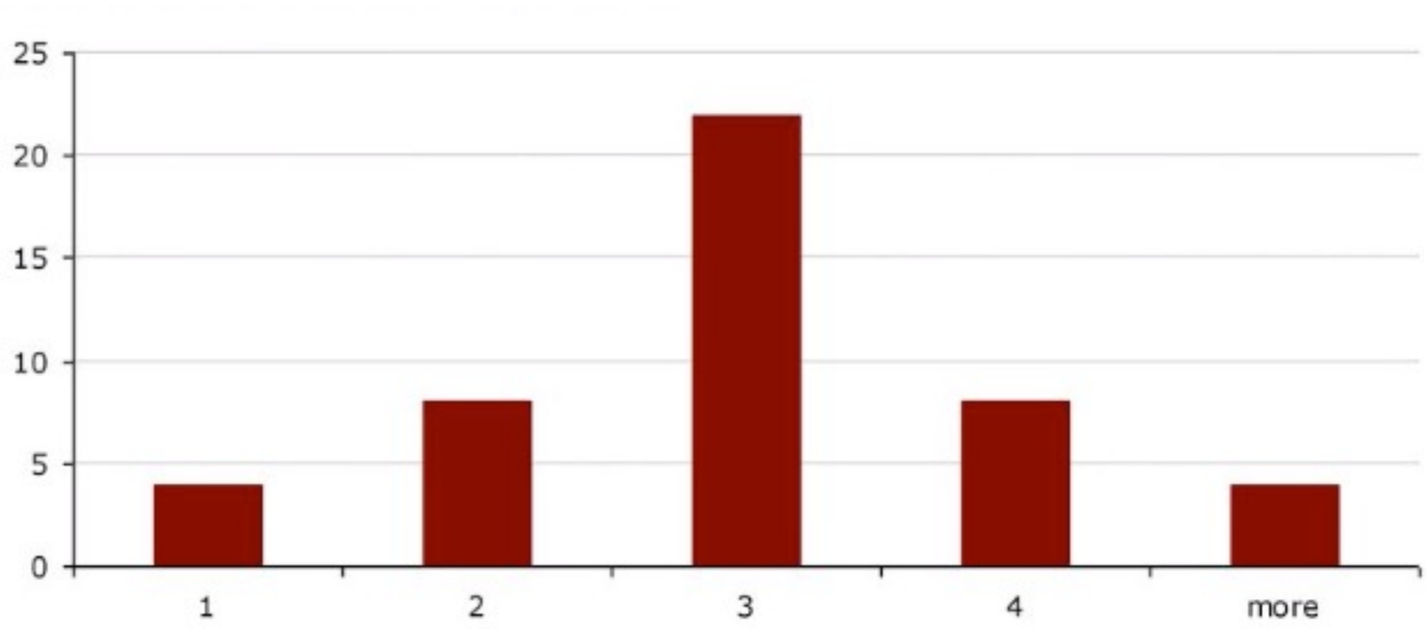
Box plot (2)

- The box plot can provide answers to the following questions:
  - Is a factor significant?
  - Does the location differ between subgroups?
  - Does the variation differ between subgroups?
  - Are there any outliers?



Skewness

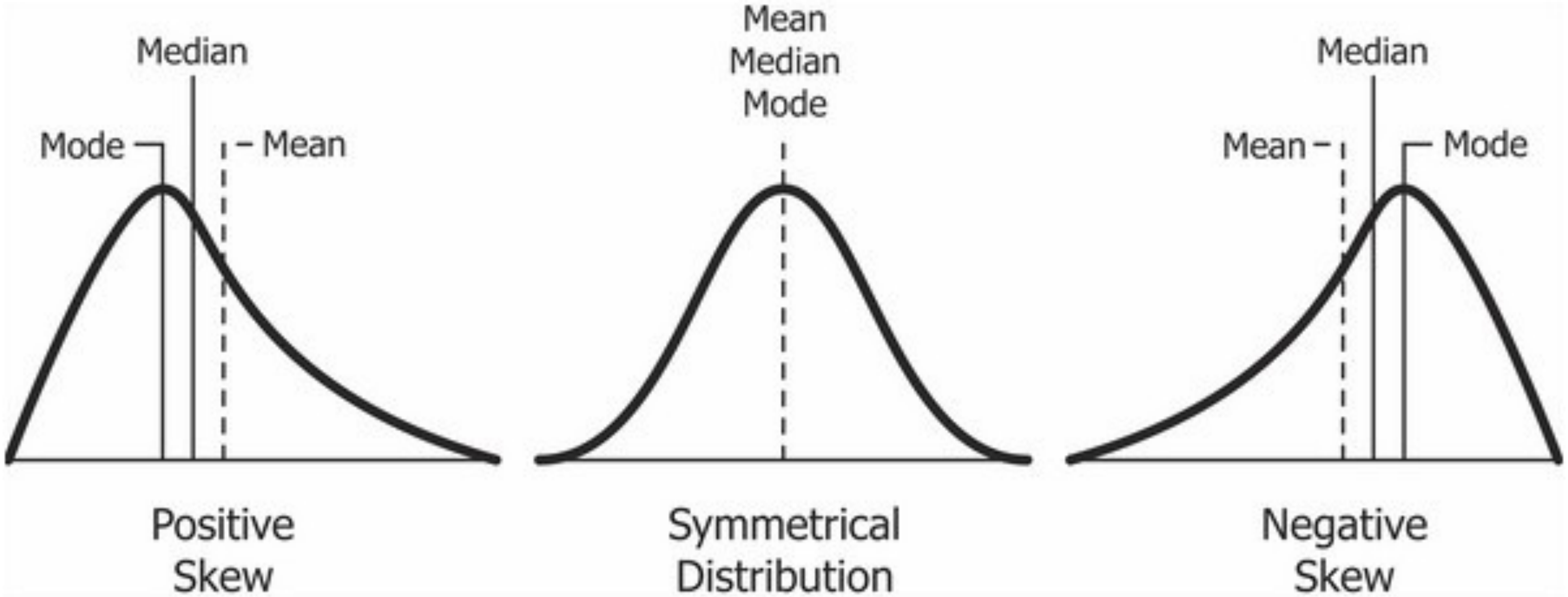
- Skewness is a measure of asymmetry. A distribution, or data set, is symmetric if it looks the same to the left and right of the center point
- Symetrical distribution



Mean = median = mode = 3

Negative, positive skewness

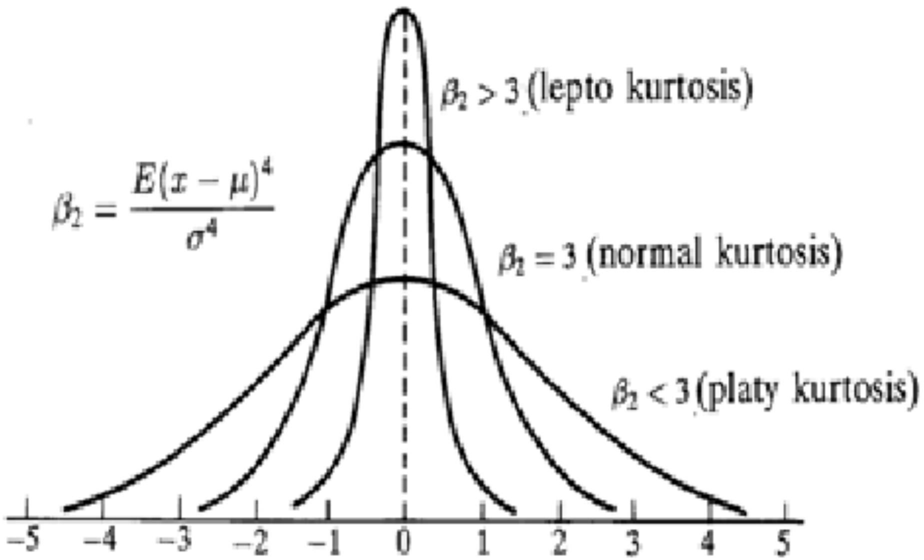
$$s_k = \frac{\sum_{i=1}^{T}\left(x_i - \bar{x}\right)^3}{\sigma^3}$$



Kurtosis

- Kurtosis is a measure of whether the data are peaked or flat relative to a normal distribution. data sets with high kurtosis tend to have a distinct peak near the mean, decline rather rapidly, and have heavy tails. Data sets with low kurtosis tend to have a flat top near the mean rather than a sharp peak.

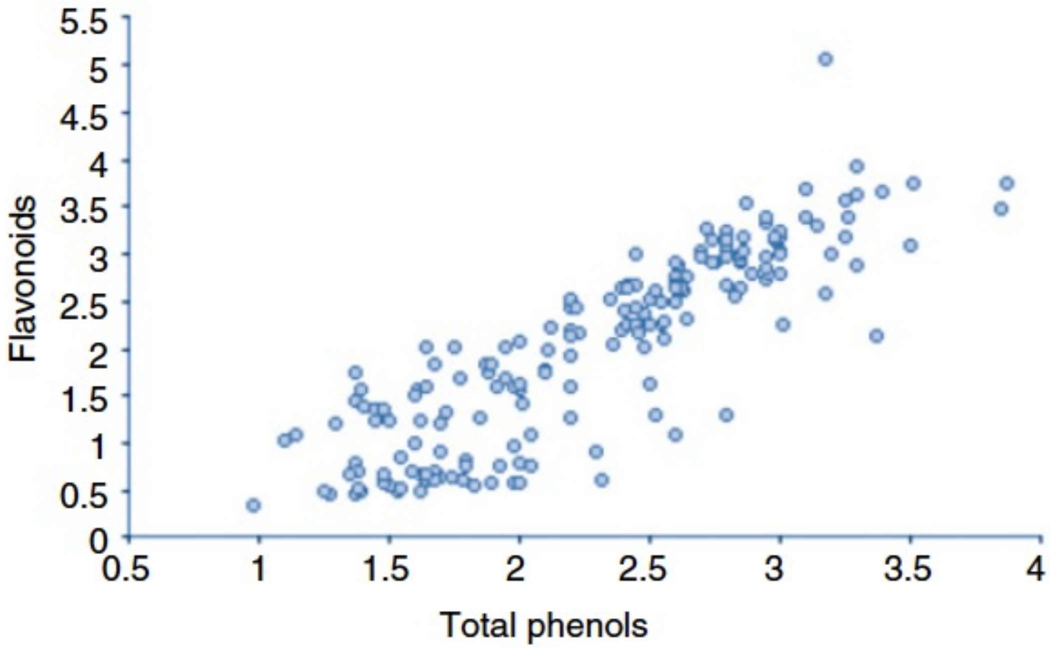
$$k = \frac{\sum_{i=1}^{T}\left(x_i - \bar{x}\right)^4}{\sigma^4}$$



Understanding relationships

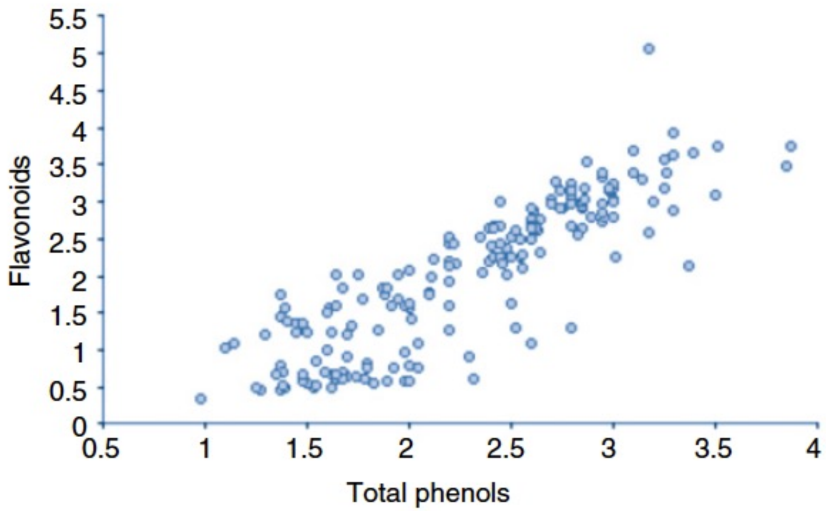
Scatter plot

- identify whether a relationship exists between two continuous variables measured on the ratio or interval scales
  - two variables are plotted on the x-and y-axis
  - each point is a single observation.

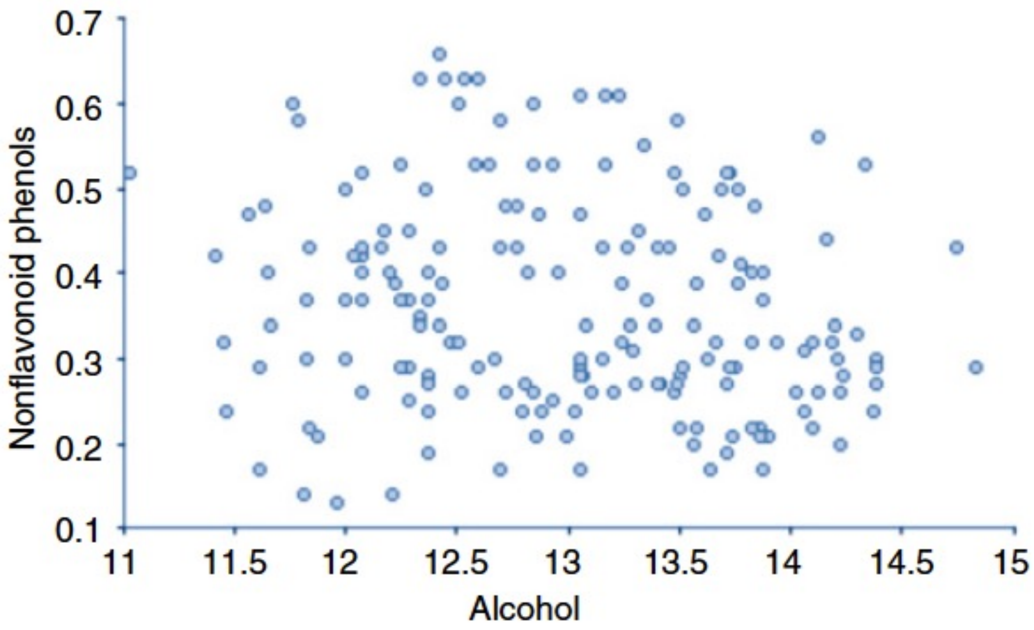


Scatter plot

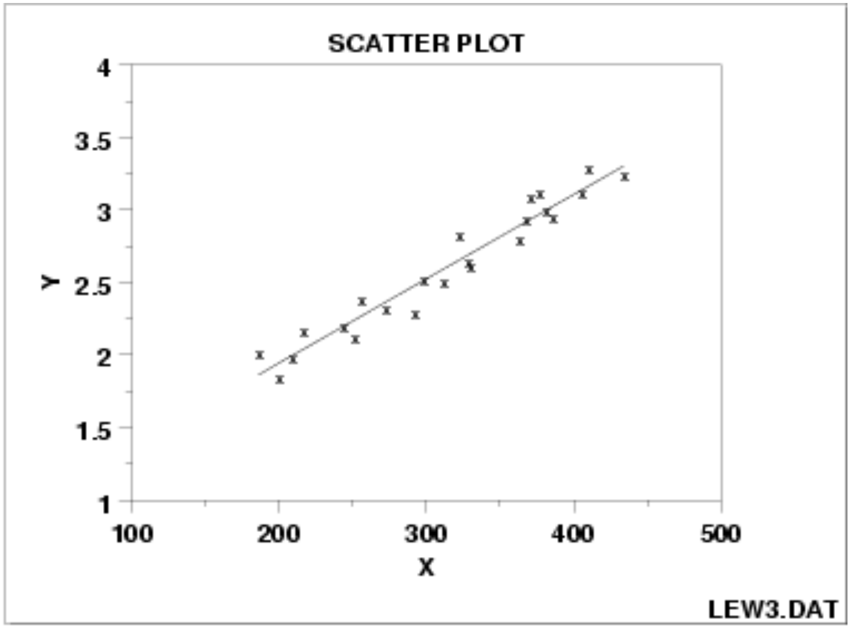
- Scatter plots can provide answers to the following questions:
  - Are variables X and Y related?
  - Are variables X and Y linearly related?
  - Are variables X and Y non-linearly related?
  - Does the variation in Y change depending on X?
  - Are there outliers?

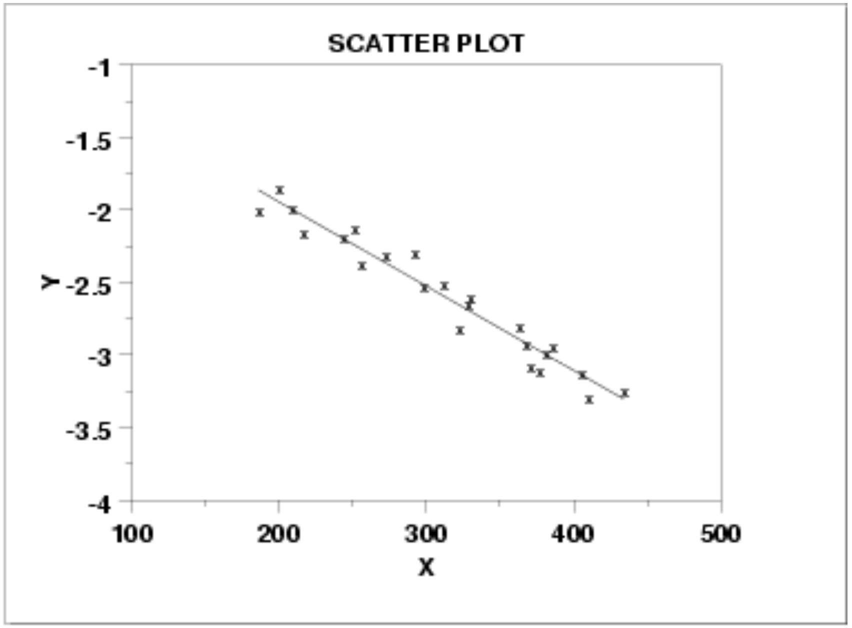


Scatter plot: No relationship

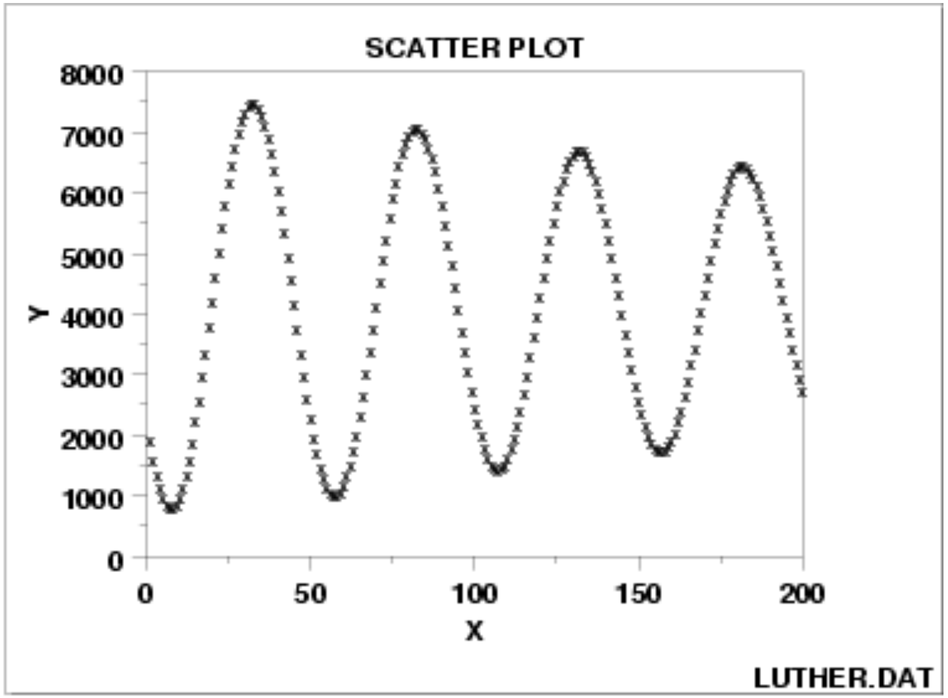


Scatter plot: Strong linear (positive - negative correlation)

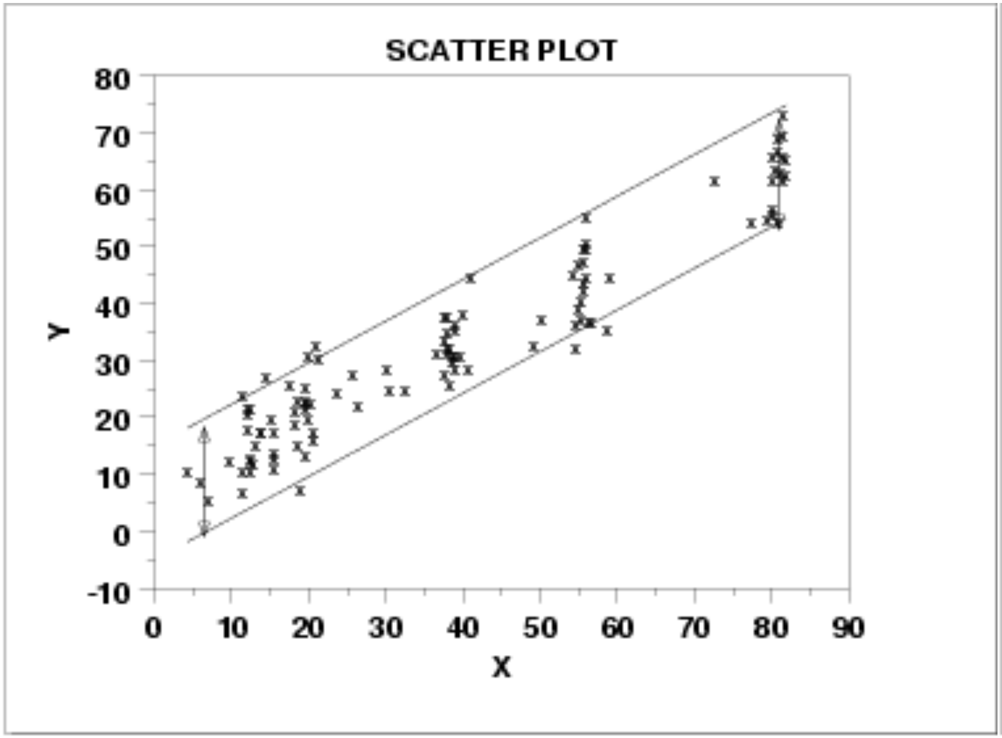


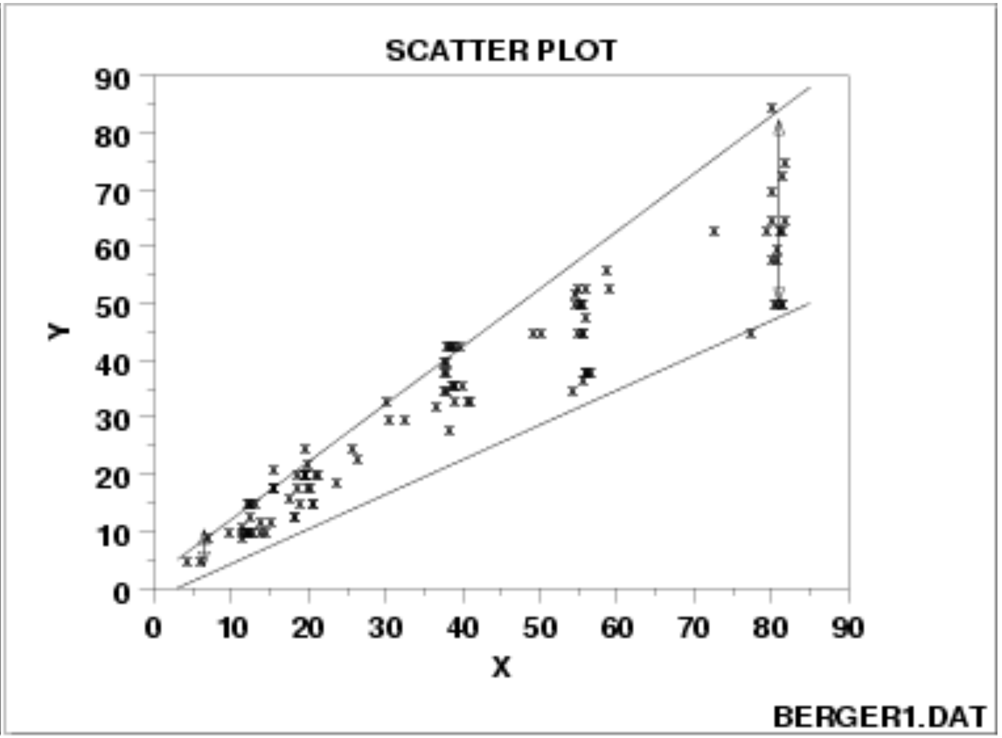


Scatter plot: Sinusoidal relationship (damped)

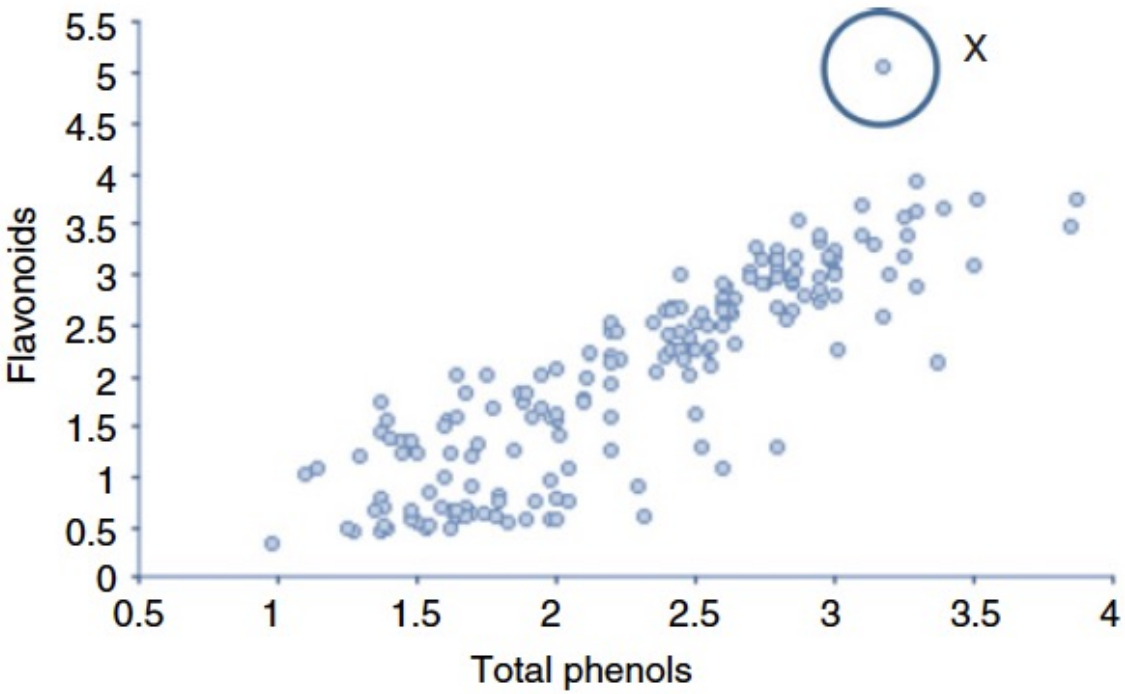


Scatter plot: variation of Y does not depend on X (homoscedastic)



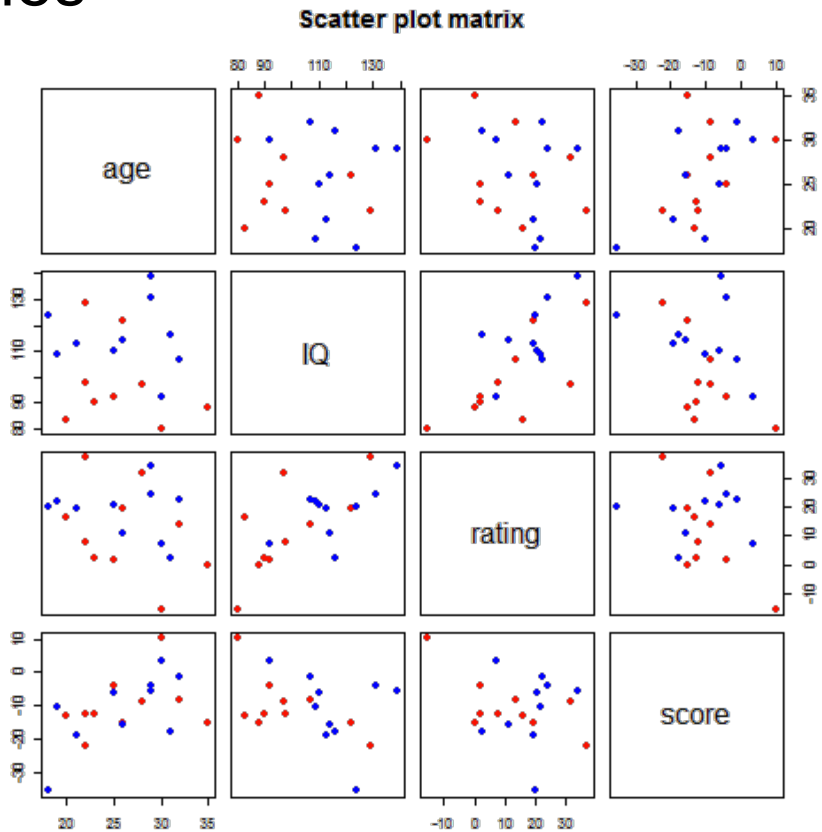


Scatter plot: Outlier



Scatterplot matrix

- a collection of **scatterplots** organized into a grid (or **matrix**).
- Each **scatterplot** shows the relationship between a pair of variables

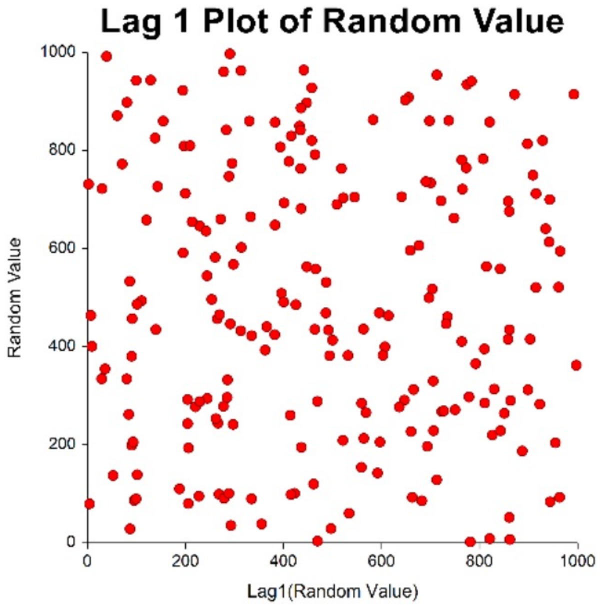


Lag plot

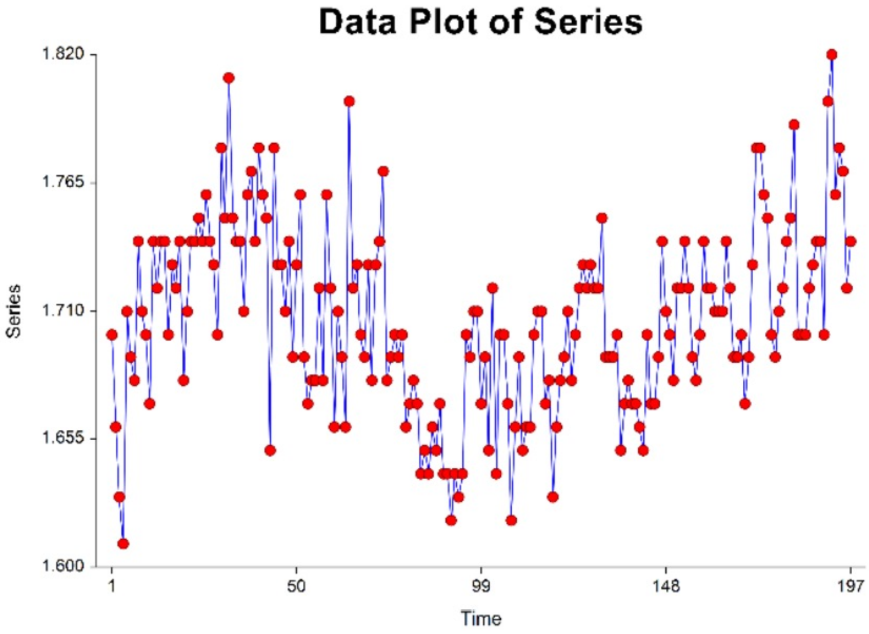
- For data values Y_1, Y_2, …, Y_N, the k-period (or k^{th}) lag of the value Y_i is defined as the data point that occurred k time points before time i. That is $\text{Lag}_k(Y_i) = Y_{i-k}$ For example, $\text{Lag}_1(Y_2) = Y_1$ and $\text{Lag}_3(Y_{10}) = Y_7$
- Lag plots can provide answers to the following questions:
  - 1. Are the data random?
  - 2. Is there serial correlation in the data?
  - 3. What is a suitable model for the data?
  - 4. Are there outliers in the data?

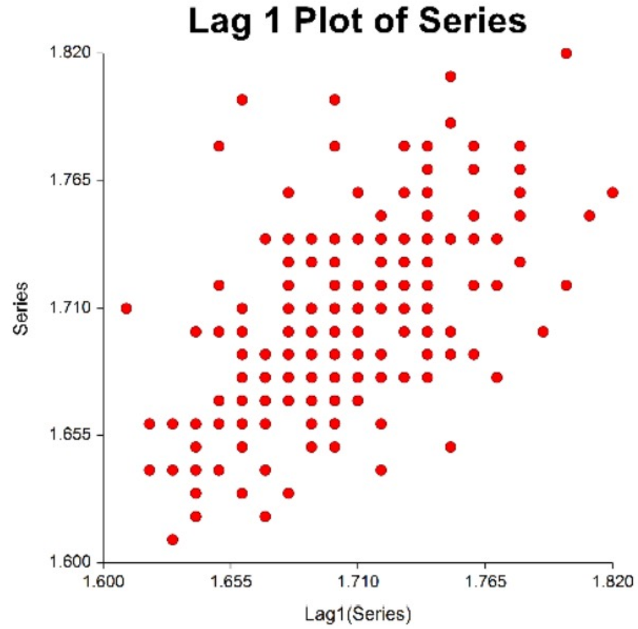
Lag plot patterns

- Random Data

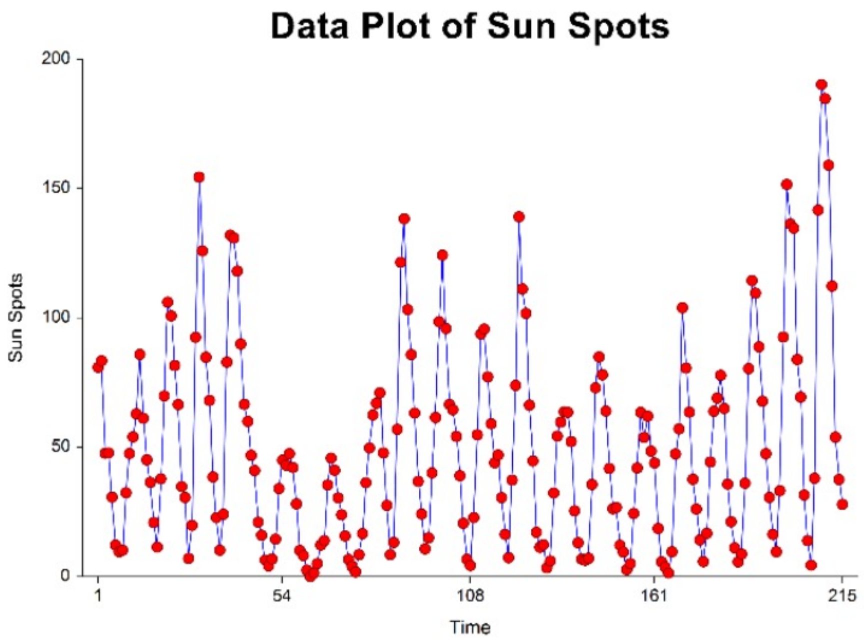


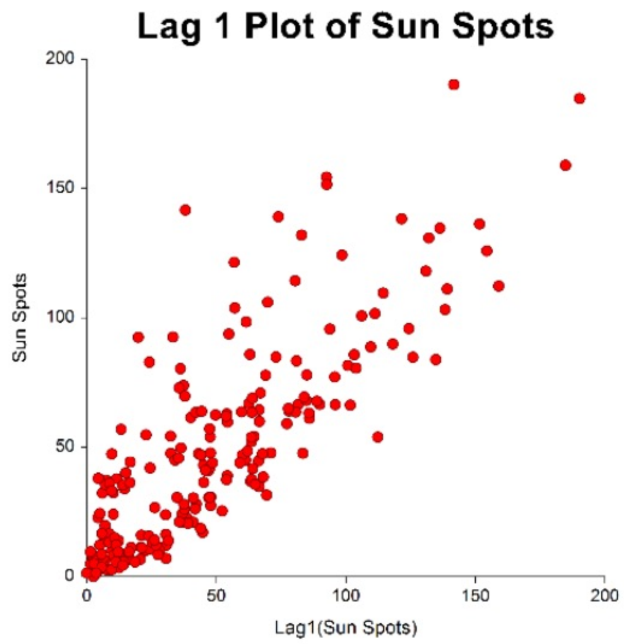
Data with weak autocorrelation



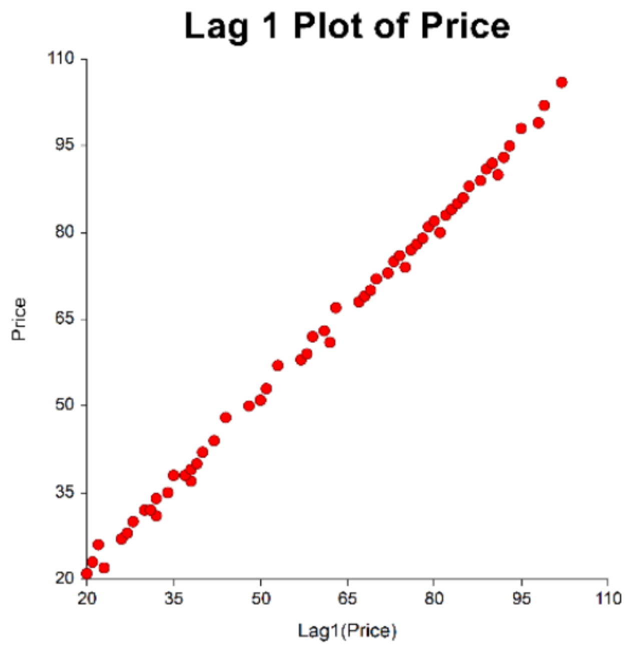


Data with moderate autocorrelation

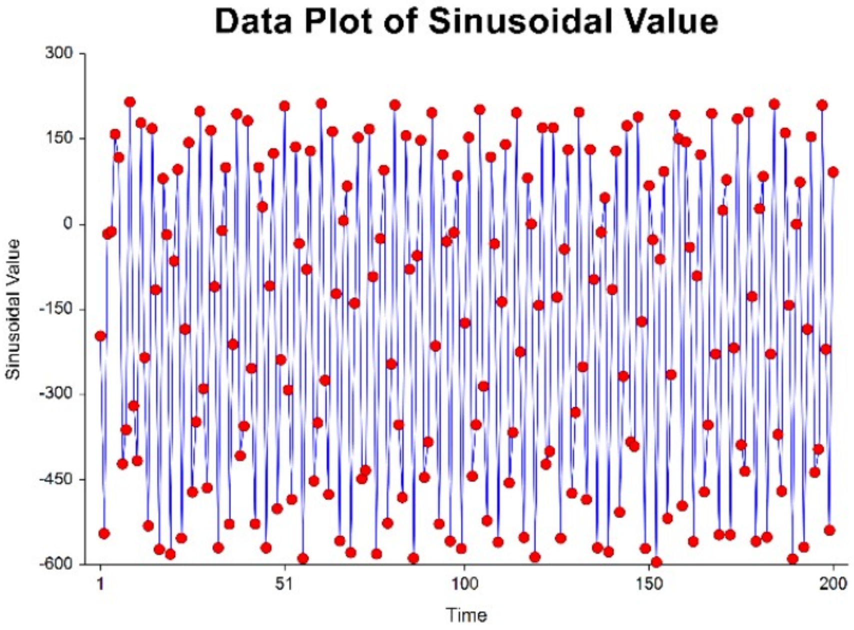


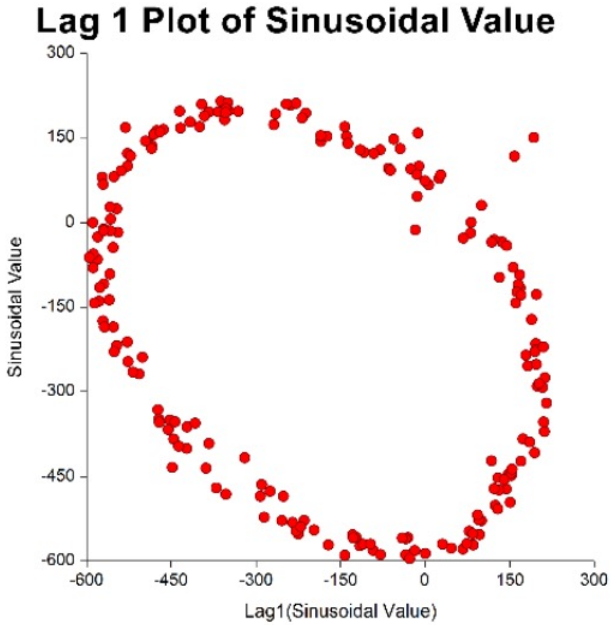


Data with high autocorrelation



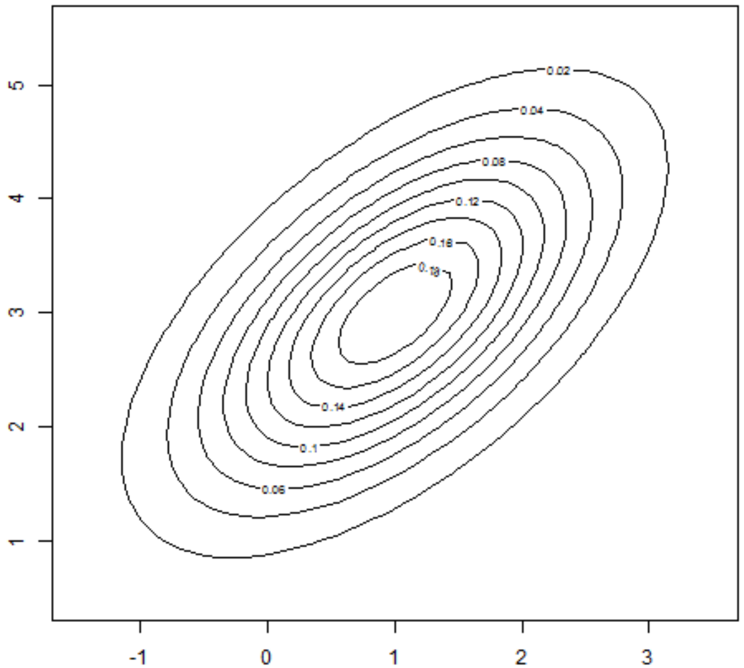
Sinusoidal data





Contour plots

- show a three-dimensional surface on a two-dimensional plane. Contour lines indicate elevations that are the same
- The contour plot is used to answer the question
  - How does Z change as a function of X and Y?



Demo

Identifing and understanding groups

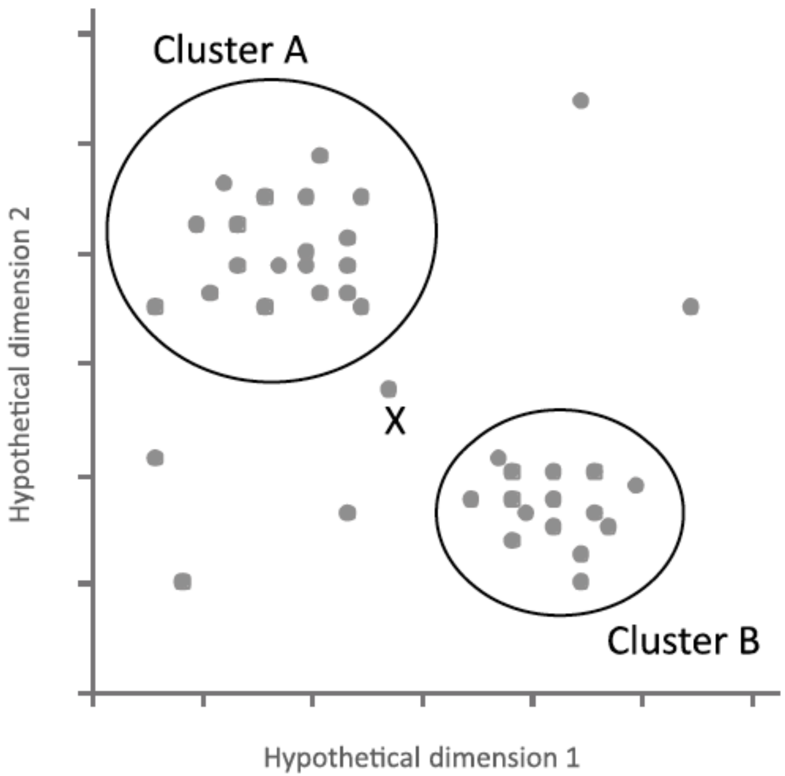
Clustering Methods in Exploratory Analysis

Motivation

- Decomposing a data set into simpler subsets helps make sense of the entire collection of observations
  - uncover relationships in the data such as groups of consumers who buy certain combinations of products
  - identify rules from the data
  - discover observations dissimilar from those in the major identified groups (possible errors or anomalies)

Clustering

- A way of grouping together data samples that are ***similar*** in some way - according to some criteria
- A form of ***unsupervised learning*** – you generally don't have examples demonstrating how the data *should* be grouped together



Can we find things that are close together?

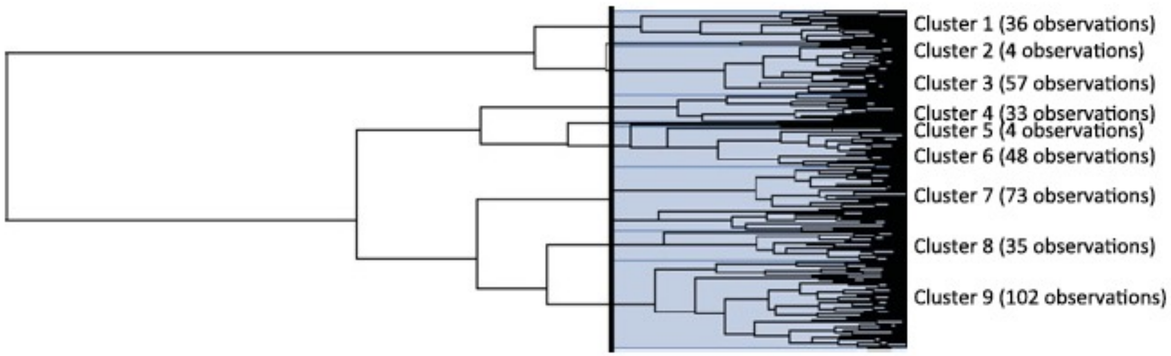
- Clustering organizes things that are close into groups
  - How do we define close?
  - How do we group things?
  - How do we visualize the grouping?
  - How do we interpret the grouping?

Types of clustering

- Hierarchical clustering
- Flat clustering

Hierarchical clustering

- An agglomerative approach
  - Find closest two things
  - Put them together
  - Find next closest
- Requires
  - A defined distance
  - A merging approach
- Produces
  - A tree showing how close things are to each other (dendrogram)



SCHO

Distances

- A method of clustering needs a way to measure how similar observations are to each other.
- Continuous - Euclidean distance
- Continuous - correlation similarity
- Binary - Manhattan distance
- Pick a distance/similarity that makes sense for the problem

Euclidean distance

$$d = \sqrt{\sum_{i=1}^{n} (p_i - q_i)^2}$$

ID	Variable 1	Variable 2	Variable 3	Variable 4	Variable 5
A	0.7	0.8	0.4	0.5	0.2
B	0.6	0.8	0.5	0.4	0.2
C	0.8	0.9	0.7	0.8	0.9

$$d_{\mathrm{A-B}} = \sqrt{(0.7-0.6)^2 + (0.8-0.8)^2 + (0.4-0.5)^2 + (0.5-0.4)^2 + (0.2-0.2)^2}$$
$$d_{\mathrm{A-B}} = 0.17$$

$$d_{\mathrm{A-C}} = \sqrt{(0.7-0.8)^2 + (0.8-0.9)^2 + (0.4-0.7)^2 + (0.5-0.8)^2 + (0.2-0.9)^2}$$
$$d_{\mathrm{A-C}} = 0.83$$

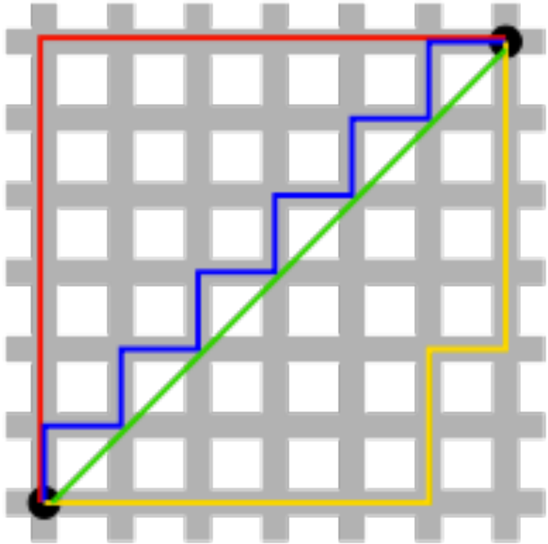
Manhattan distance

- is the sum of the lengths of the projections of the line segment between the points onto t

$$d_1(\mathbf{p}, \mathbf{q}) = \|\mathbf{p} - \mathbf{q}\|_1 = \sum_{i=1}^{n} |p_i - q_i|,$$

where $(\mathbf{p}, \mathbf{q})$ are vectors

$$\mathbf{p} = (p_1, p_2, \dots, p_n) \text{ and } \mathbf{q} = (q_1, q_2, \dots, q_n)$$

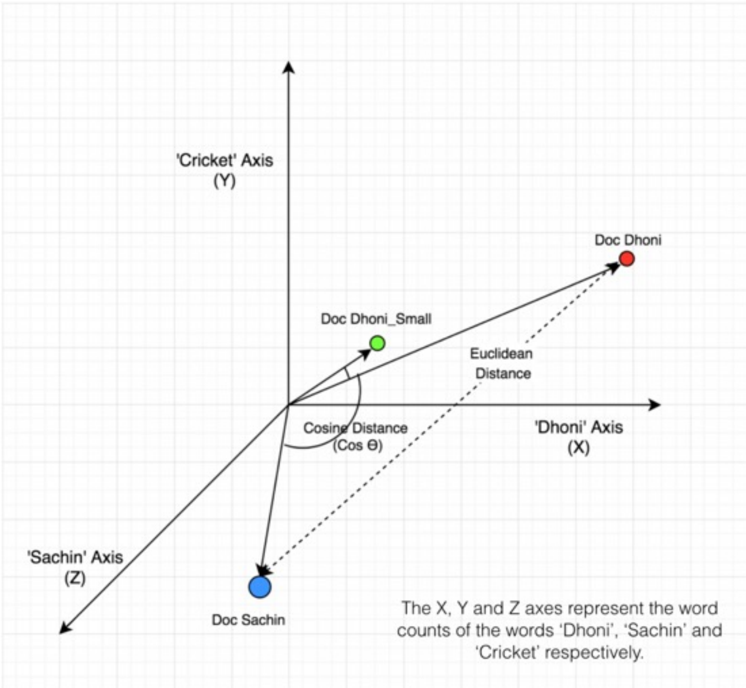


Cosine distance

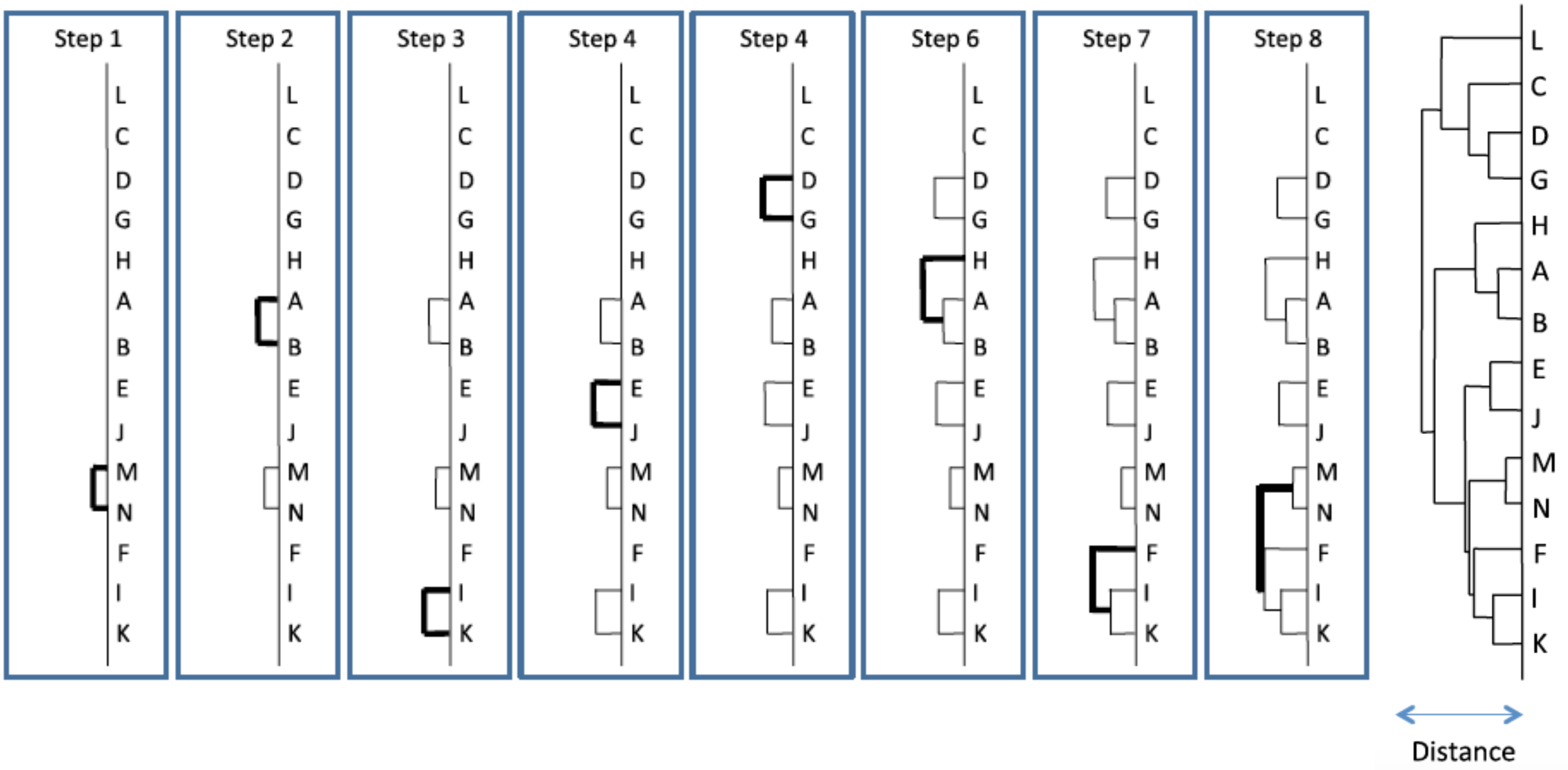
$$Cos\theta = \frac{\vec{a} \cdot \vec{b}}{\|\vec{a}\| \, \|\vec{b}\|} = \frac{\sum_1^n a_i b_i}{\sqrt{\sum_1^n a_i^2} \sqrt{\sum_1^n b_i^2}}$$

where, $\vec{a} \cdot \vec{b} = \sum_1^n a_i b_i = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n$ is the dot product of the two vectors.

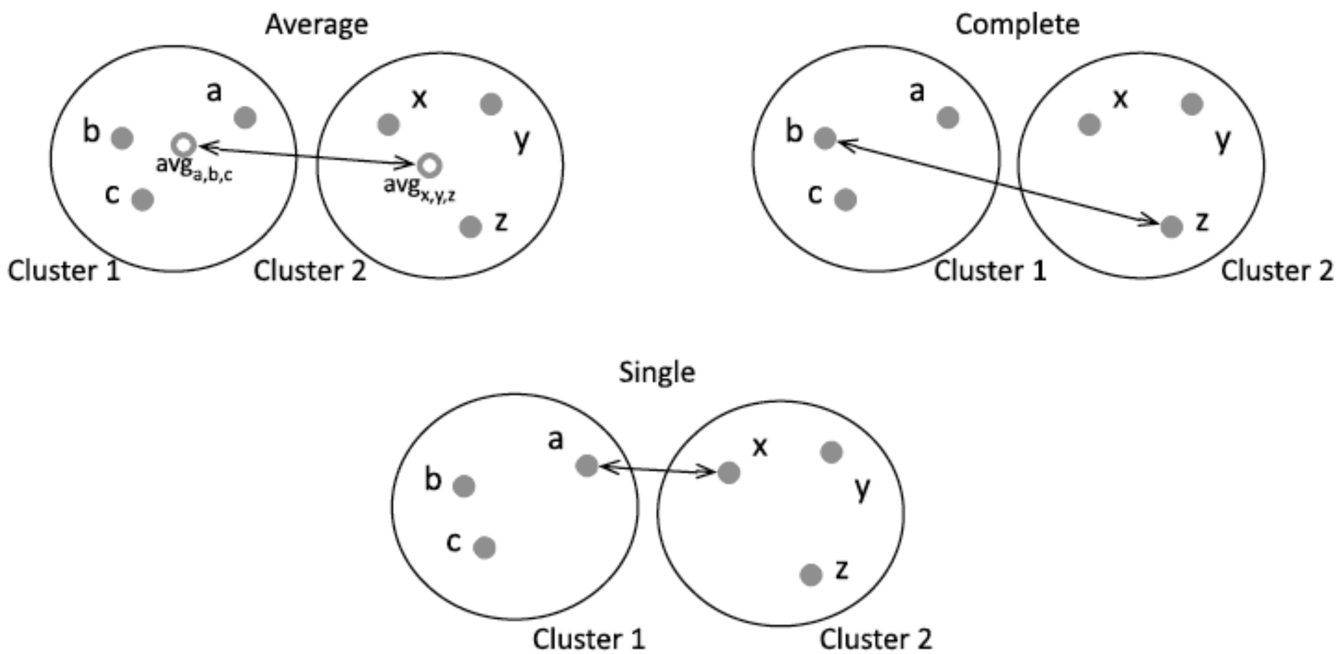
Projection of Documents in 3D Space



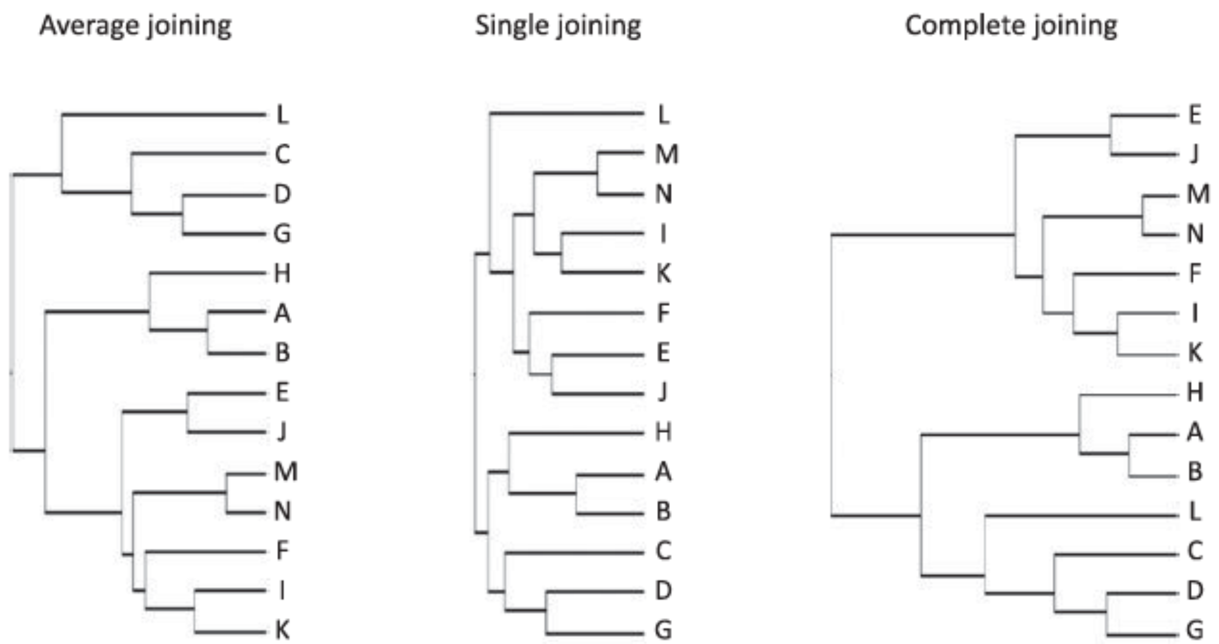
Agglomerative Hierarchical Clustering Algorithm



Linkage rules



AHC result


Average joining
L
C
D
G
H
A
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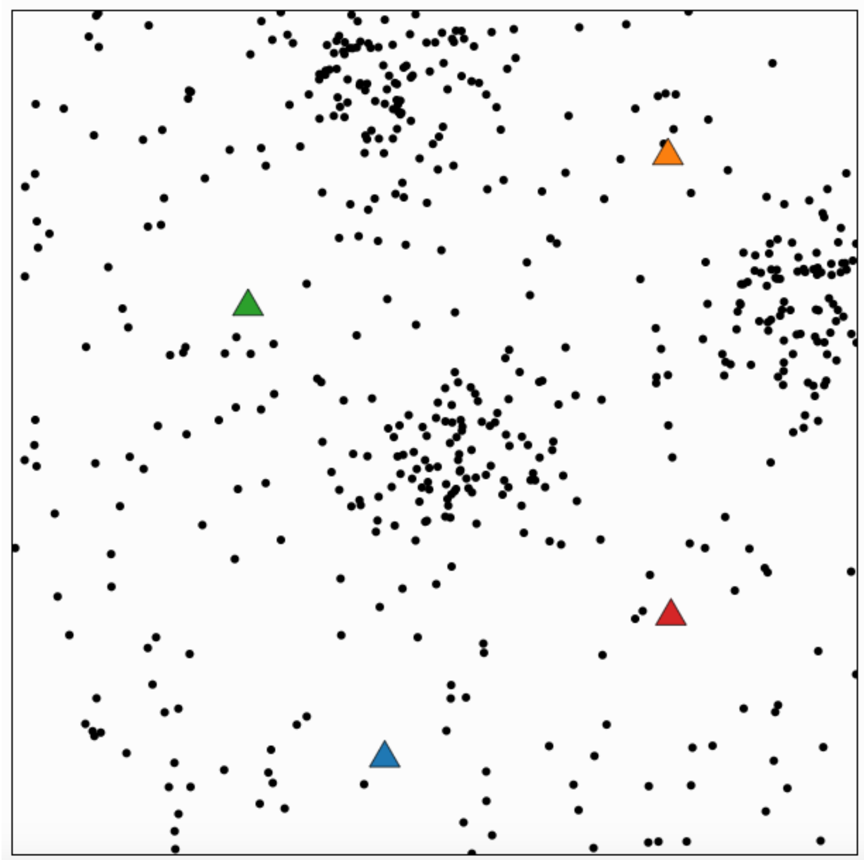
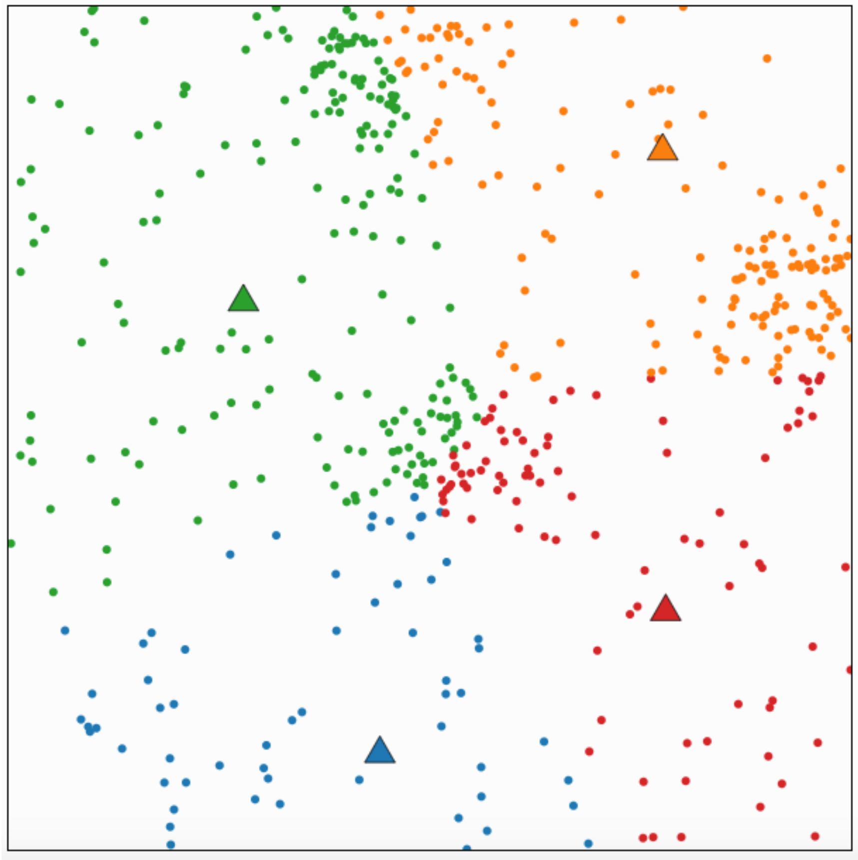
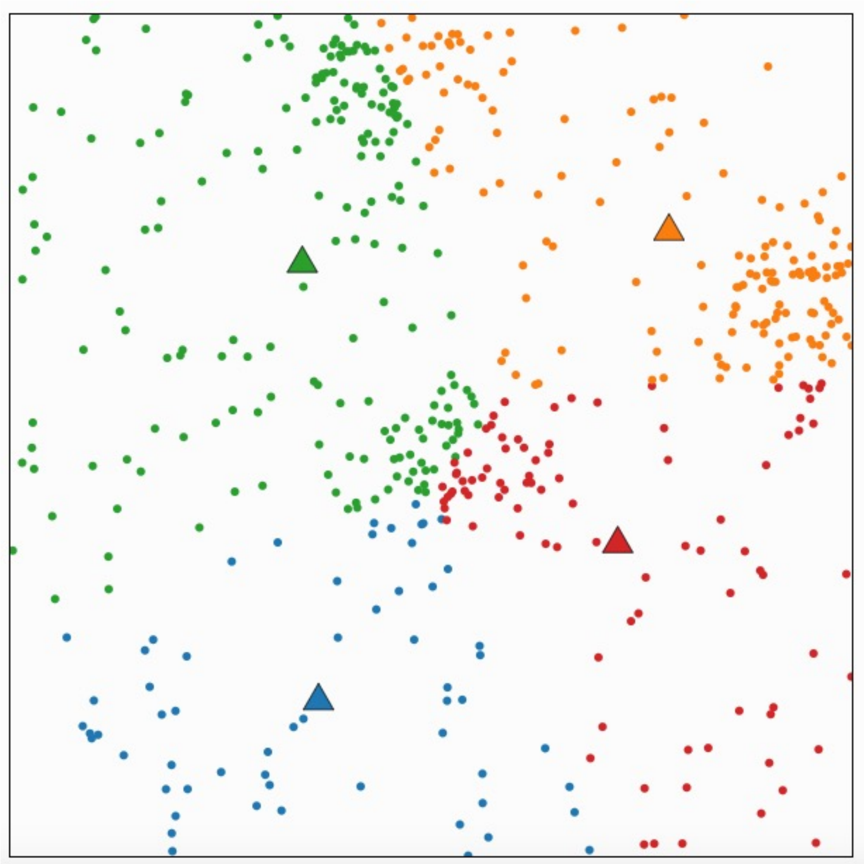
M
N
F
I
K
Single joining
L
M
N
I
K
F
E
J
H
A
B
C
D
G
Complete joining
E
J
M
N
F
I
K
H
A
B
L
C
D
G

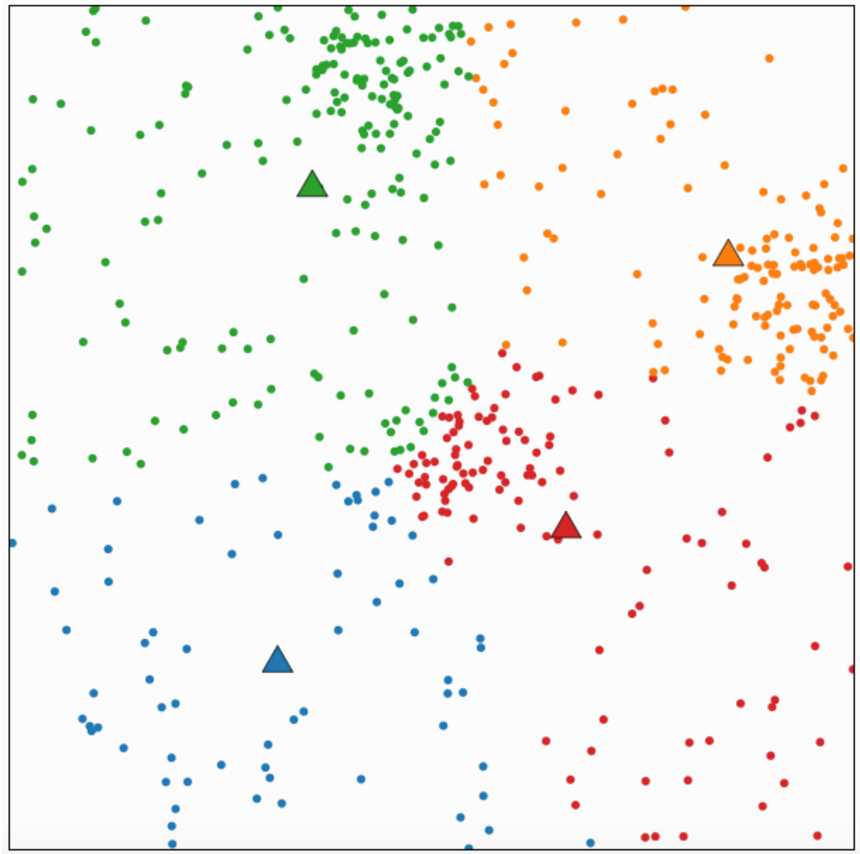
K-mean clustering

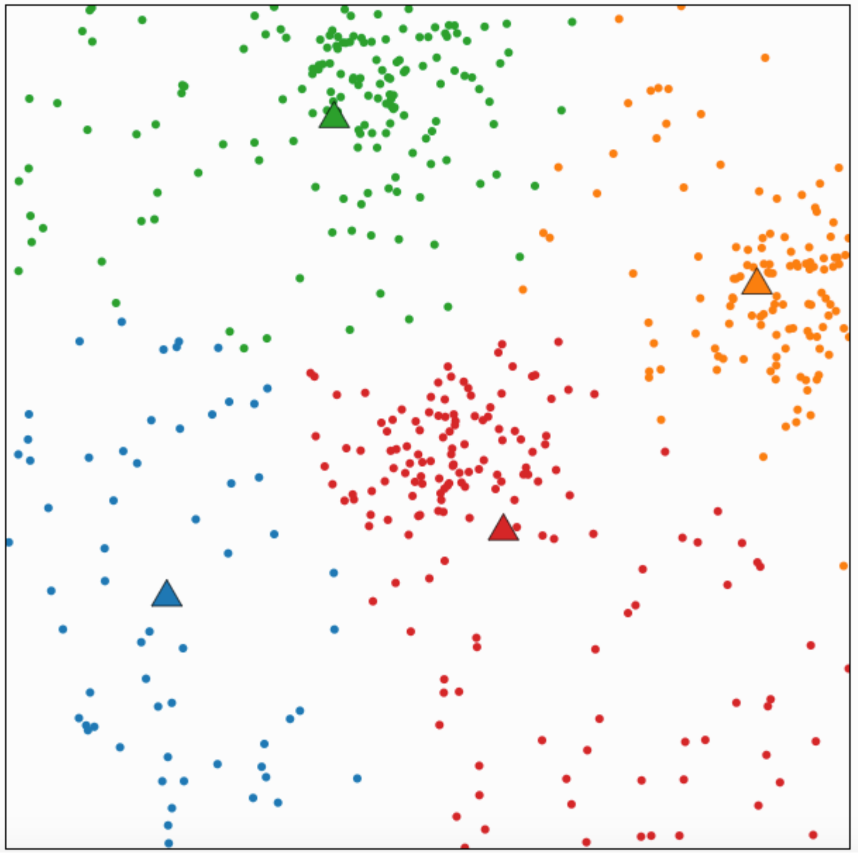
- A partitioning approach
  - Fix a number of clusters
  - Get “centroids” of each cluster
  - Assign things to closest centroid
  - Recalculate centroids
- Requires
  - A defined distance metric
  - A number of clusters
  - An initial guess as to cluster centroids
- Produces
  - Final estimate of cluster centroids
  - An assignment of each point to clusters











Dimensionality reduction

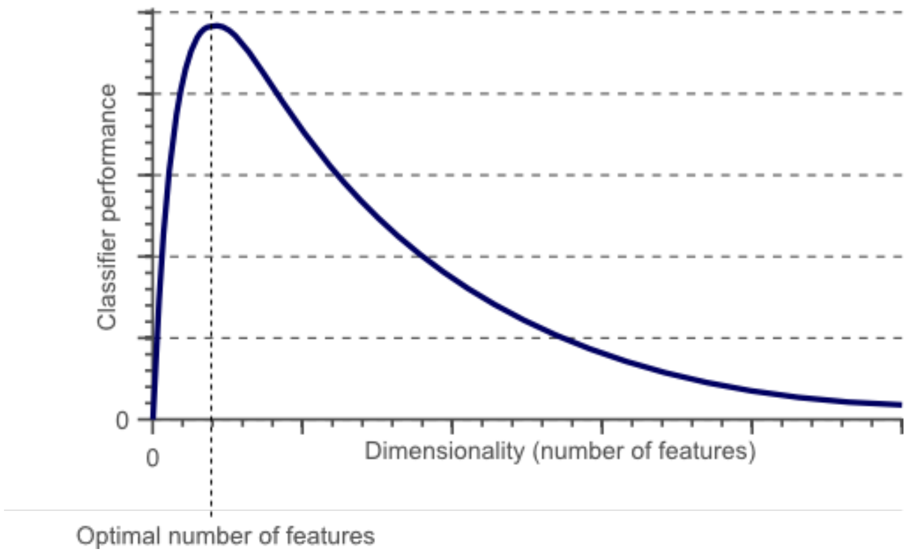
Principal Components Analysis and Singular Value Decomposition

Motivation

- Most machine learning and data mining techniques may not be effective for high-dimensional data
  - Curse of Dimensionality. Irrelevant and redundant features can “confuse” learners!
  - The intrinsic dimension may be small.

Curse of dimensionality

- The required number of samples (to achieve the same accuracy) grows exponentionally with the number of variables!
- In practice: number of training examples is fixed!
  - => the classifier's performance usually will degrade for a large number of features!

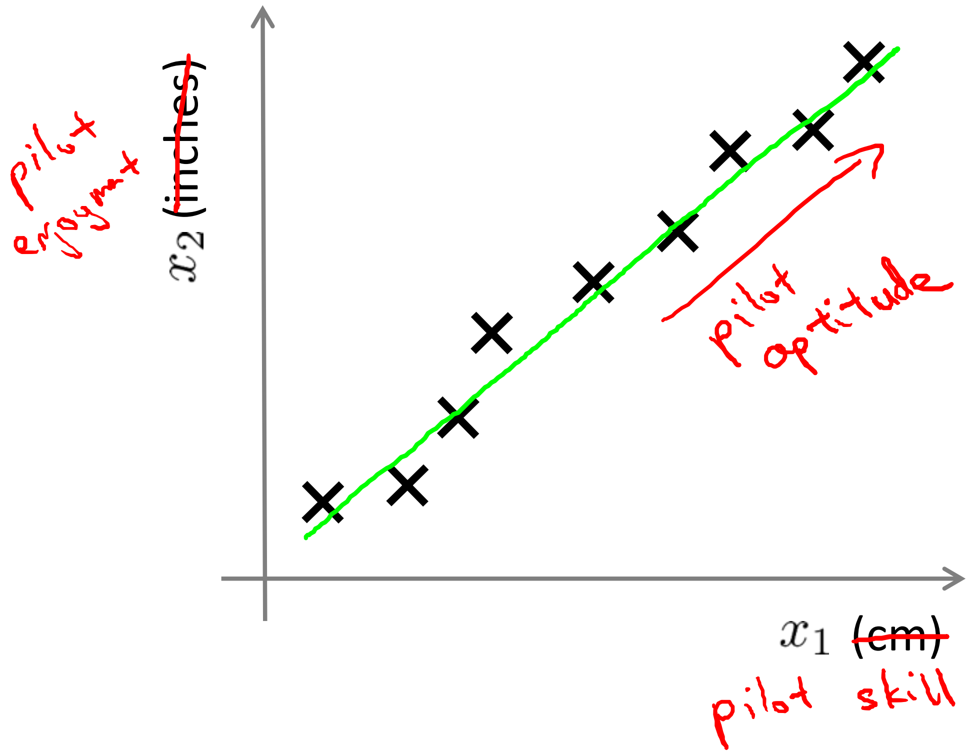


After a certain point, increasing the dimensionality of the problem by adding new features would actually degrade the performance of classifier.

Motivation

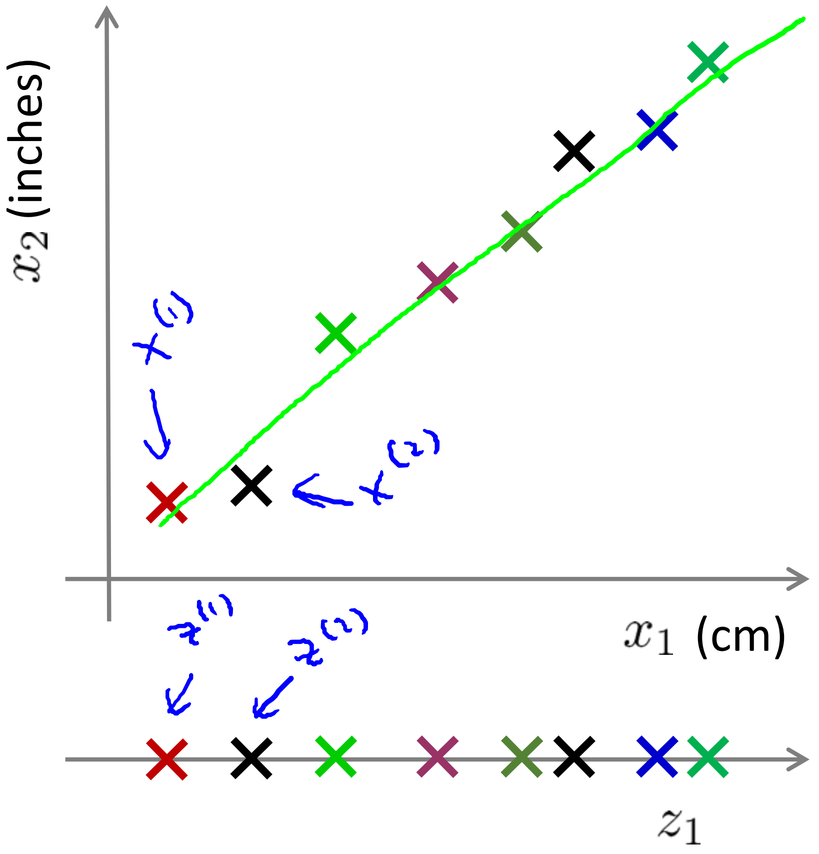
- Dimensionality reduction is an effective approach to downsizing data
  - Visualization: projection of high-dimensional data onto 2D or 3D.
  - Data compression: efficient storage and retrieval.
  - Noise removal: positive effect on query accuracy.

Data compression



Reduce data from 2D to 1D

Data compression (2)



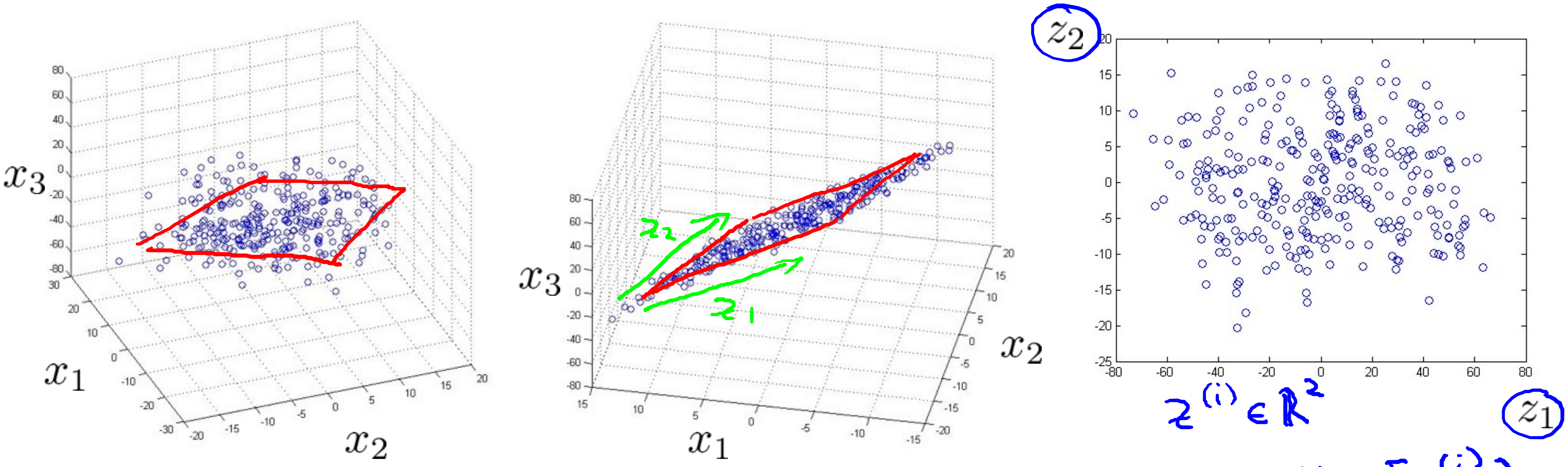
Reduce data from 2D to 1D

$$x^{(1)} \in \mathbb{R}^2 \quad \rightarrow z^{(1)} \in \mathbb{R}$$
$$x^{(2)} \in \mathbb{R}^2 \quad \rightarrow z^{(2)} \in \mathbb{R}$$
$$\vdots$$
$$x^{(m)} \in \mathbb{R}^2 \quad \rightarrow z^{(m)} \in \mathbb{R}$$

Data compression (2)

1000D → 100D

Reduce data from 3D to 2D

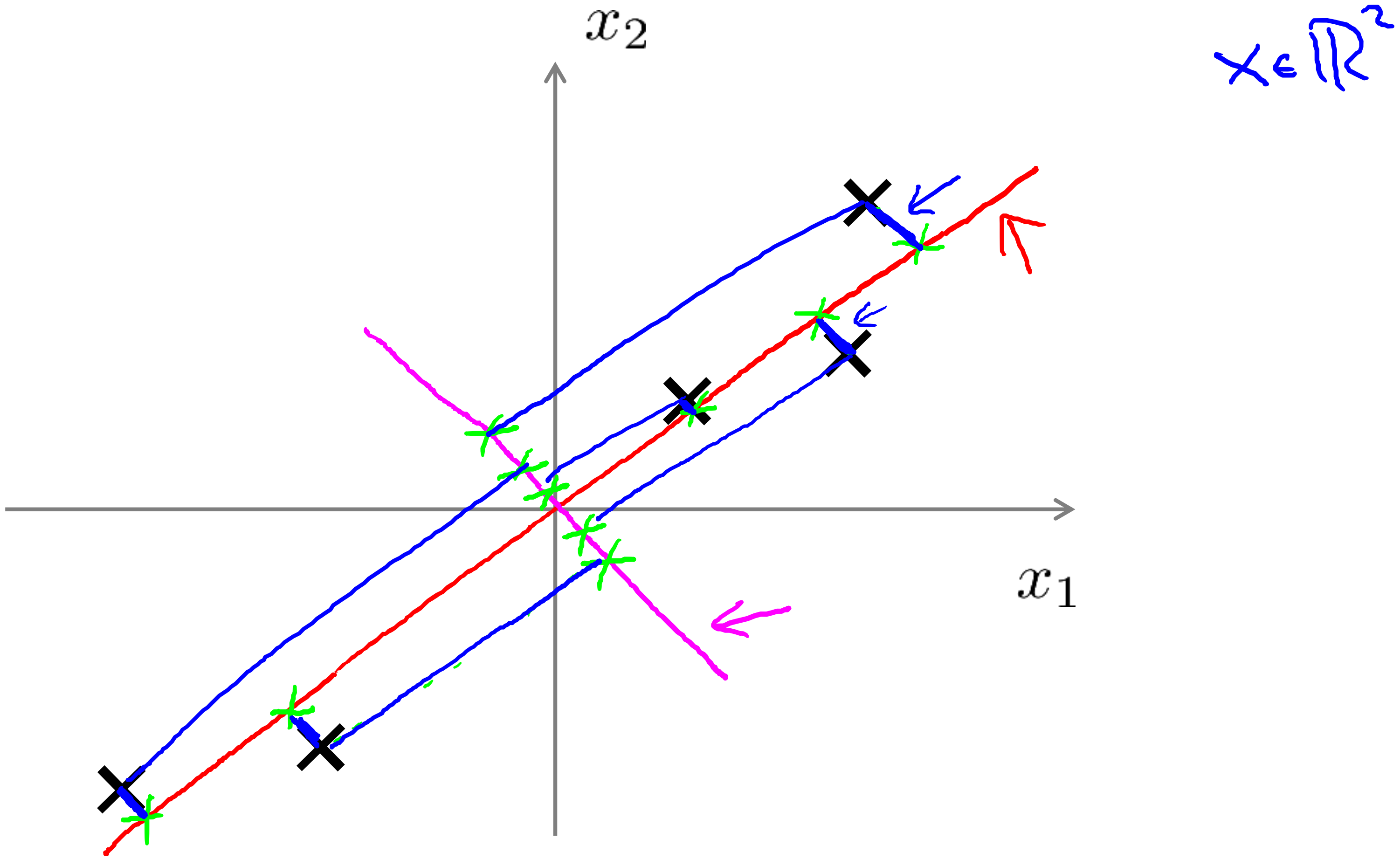


$x^{(i)} \in \mathbb{R}^3$

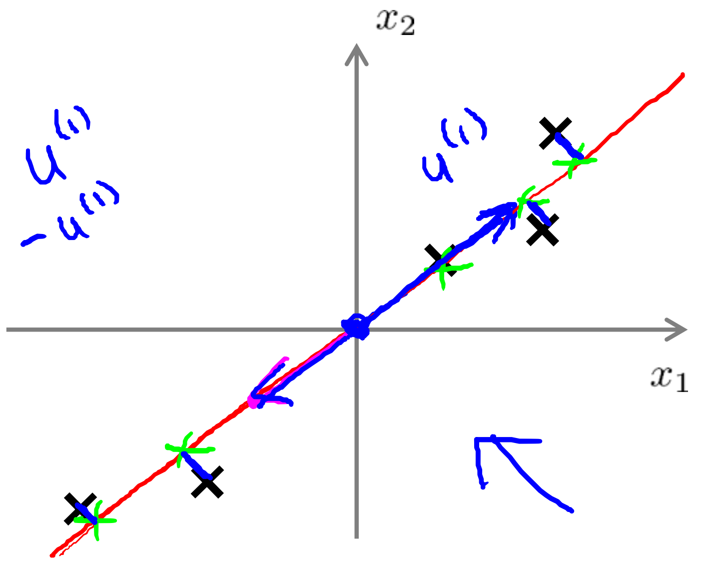
$z^{(i)} \in \mathbb{R}^2$

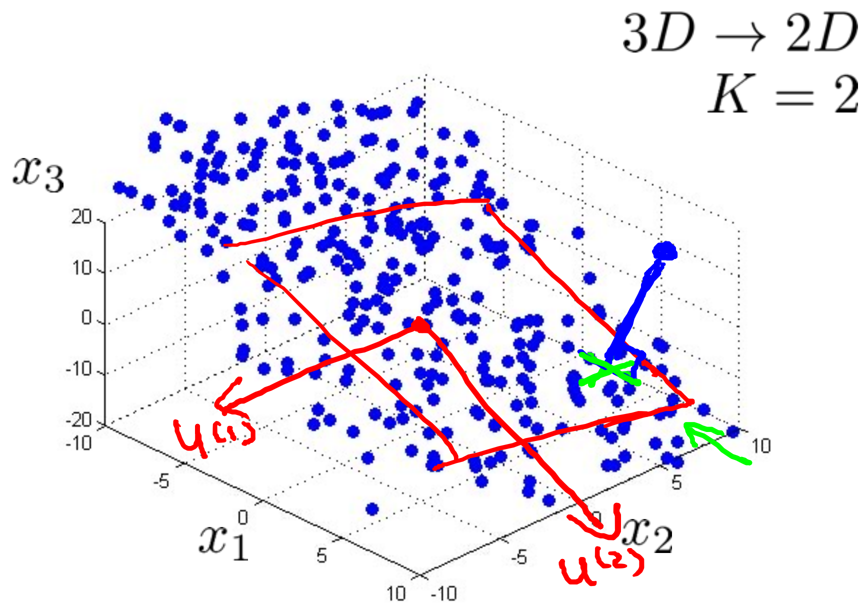
$z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$ $\quad z^{(i)} = \begin{bmatrix} z_1^{(i)} \\ z_2^{(i)} \end{bmatrix}$

Principal Component Analysis (PCA) problem formulation



Principal Component Analysis (PCA) problem formulation



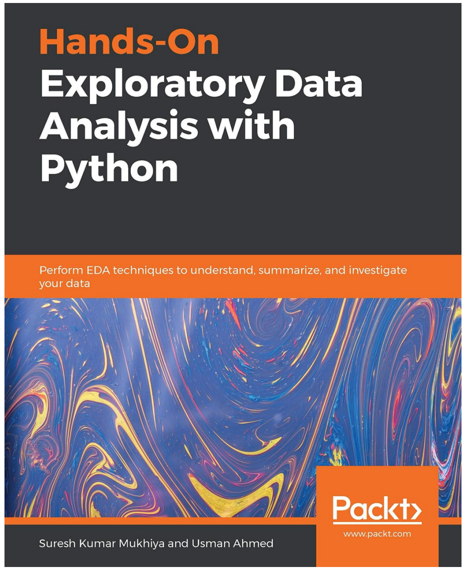


Reduce from 2-dimension to 1-dimension: Find a direction (a vector $u^{(1)} \in \mathbb{R}^n$) onto which to project the data so as to minimize the projection error.

Reduce from n-dimension to k-dimension: Find k vectors $u^{(1)}, u^{(2)}, \ldots, u^{(k)}$ onto which to project the data, so as to minimize the projection error.

Demo

References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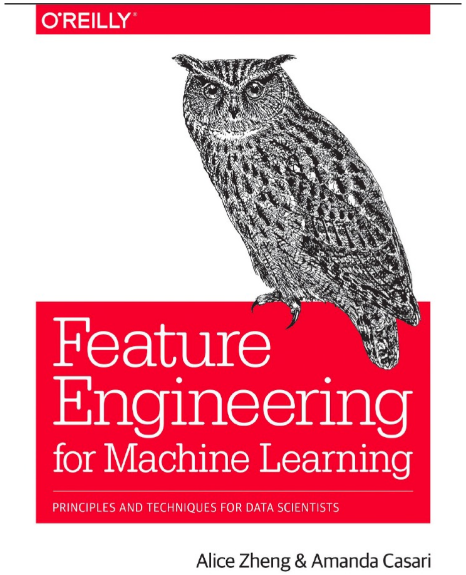
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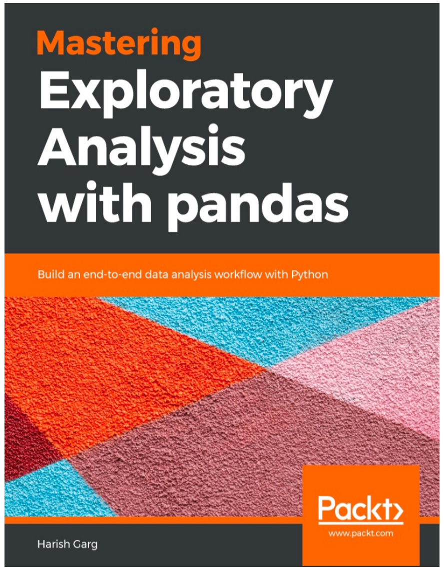
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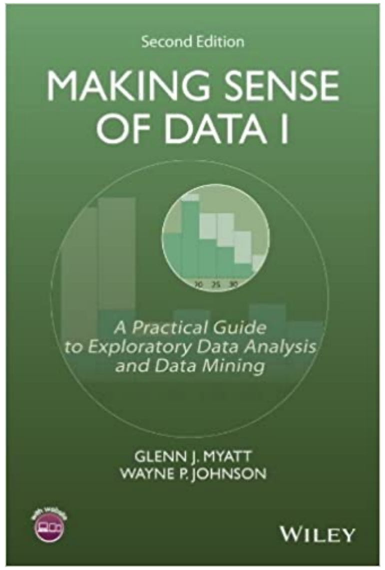
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