

# MACHINE LEARNING

## Module 1

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### Exploratory Data Analysis *(a gentle introduction)*

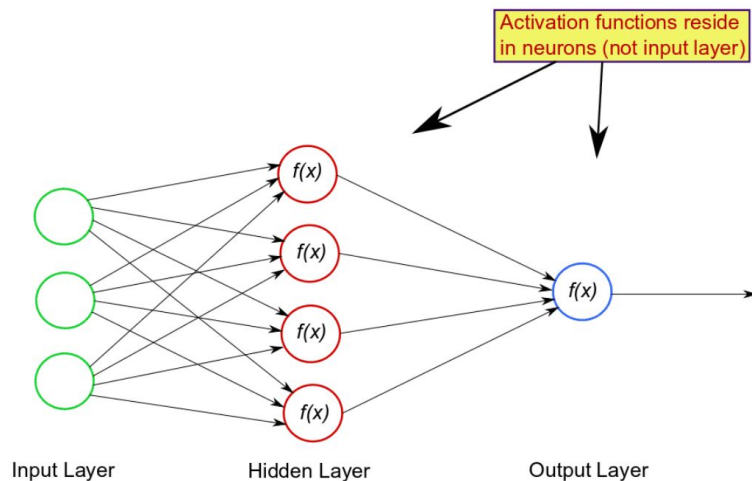
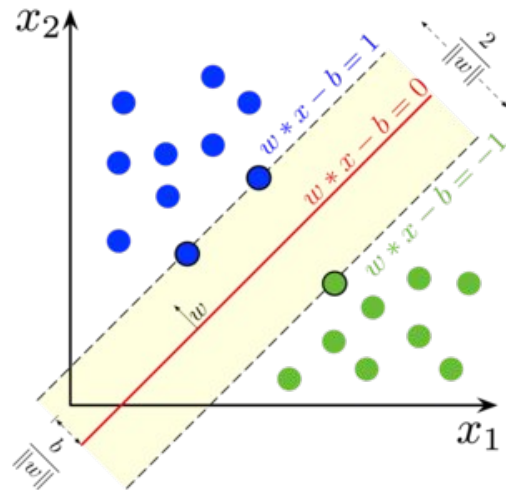
# Universal Approximation Theorem - Kurt Hornik & George Cybenko

- Artificial Neural Networks:

- non linearity
- limits
- continue

- Support Vector Machine

- Gaussian Kernel
- 



- ... others (Decision Tree, Polynomials)

# No Free Lunch Theorem - D. H. Wolpert & W. G. Macready

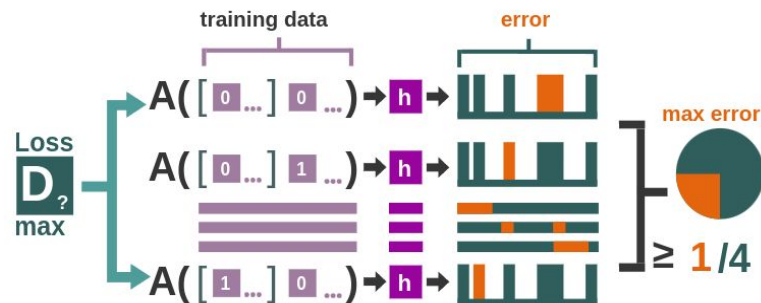
- The Core Concept

- Implications in ML

- Diversity of ML Problems

- Algorithm Selection

- Final Reflection



## No Free Lunch Theorems for Optimization

David H. Wolpert  
IBM Almaden Research Center  
N5Na/D3  
650 Harry Road  
San Jose, CA 95120-6099

William G. Macready  
Santa Fe Institute  
1399 Hyde Park Road  
Santa Fe, NM, 87501

December 31, 1996



### Abstract

A framework is developed to explore the connection between effective optimization algorithms and the problems they are solving. A number of “no free lunch” (NFL) theorems are presented that establish that for any algorithm, any elevated performance over one class of problems is exactly paid for in performance over another class. These theorems result in a geometric interpretation of what it means for an algorithm to be well suited to an optimization problem. Applications of the NFL theorems to information theoretic aspects of optimization and benchmark measures of performance are also presented. Other issues addressed are time-varying optimization problems and *a priori* “head-to-head” minimax distinctions between optimization algorithms, distinctions that can obtain despite the NFL theorems’ enforcing of a type of uniformity over all algorithms.

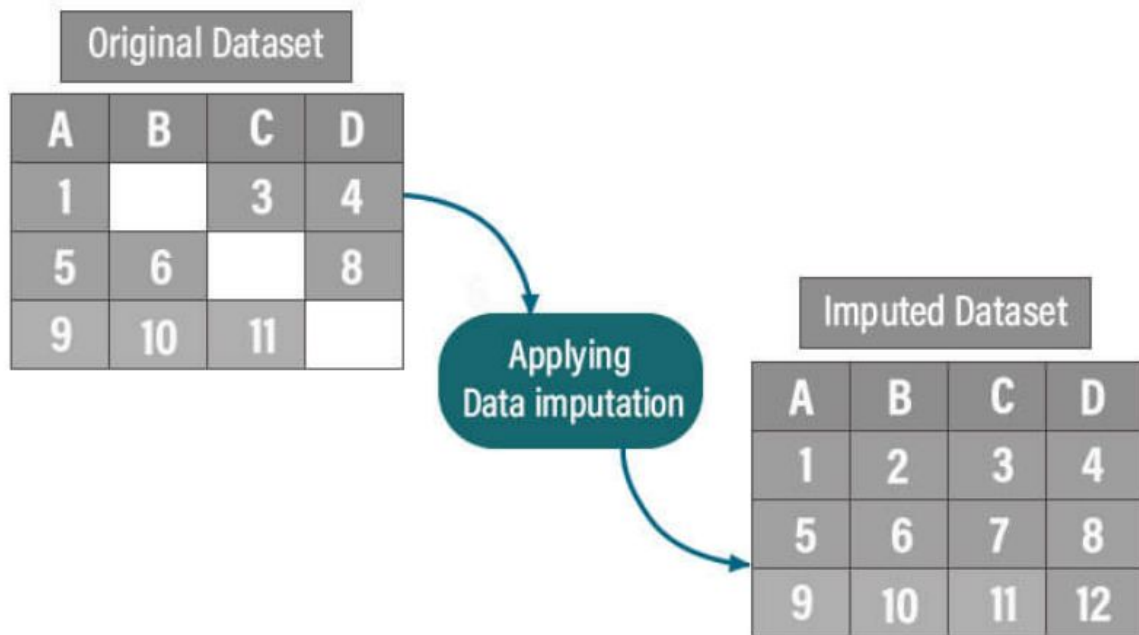
## 1 Introduction

The past few decades have seen increased interest in general-purpose “black-box” optimization algorithms that exploit little if any knowledge concerning the optimization problem on which they are run. In large part these algorithms have drawn inspiration from optimization processes that occur in nature. In particular, the two most popular black-box optimization strategies, evolutionary algorithms [FOW66, Hol93] and simulated annealing [KGW83] mimic processes in natural selection and statistical mechanics respectively.

# Module 1: Imputation

- Missing Values
- Why it is important
  - data retention
  - Performance improving
  - data preparation
- Different Strategies
  - univariate, multivariate
  - statistical, MICE, ...

## Data Imputation



# Module 1: Imputation

- mean/median/mode

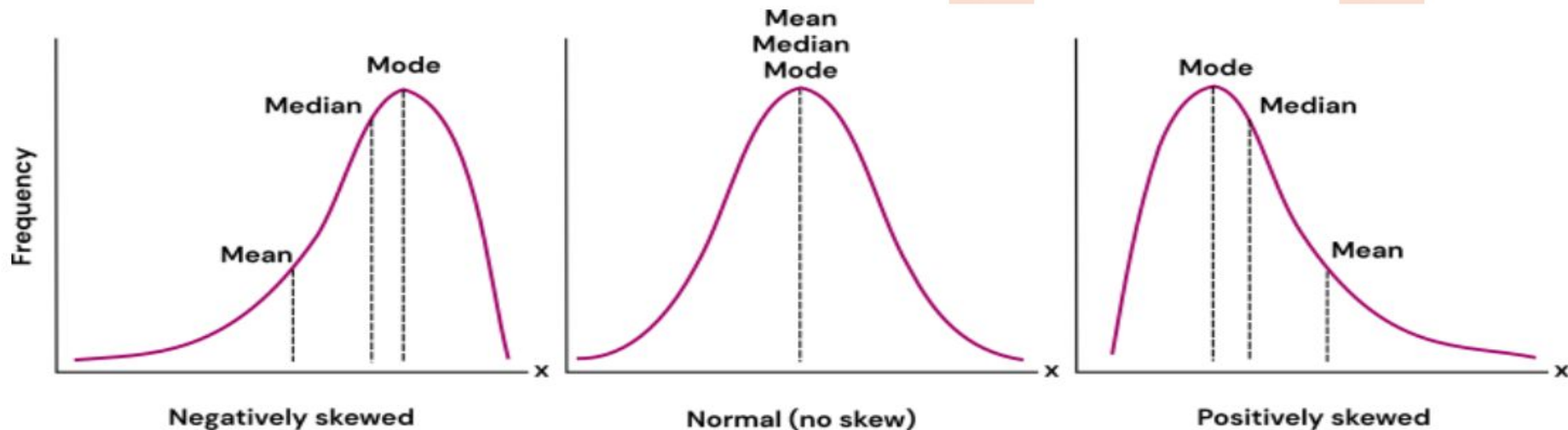
Price
100
90
50
40
20
100
60
120
200

Mean = 86.66

Median = 90

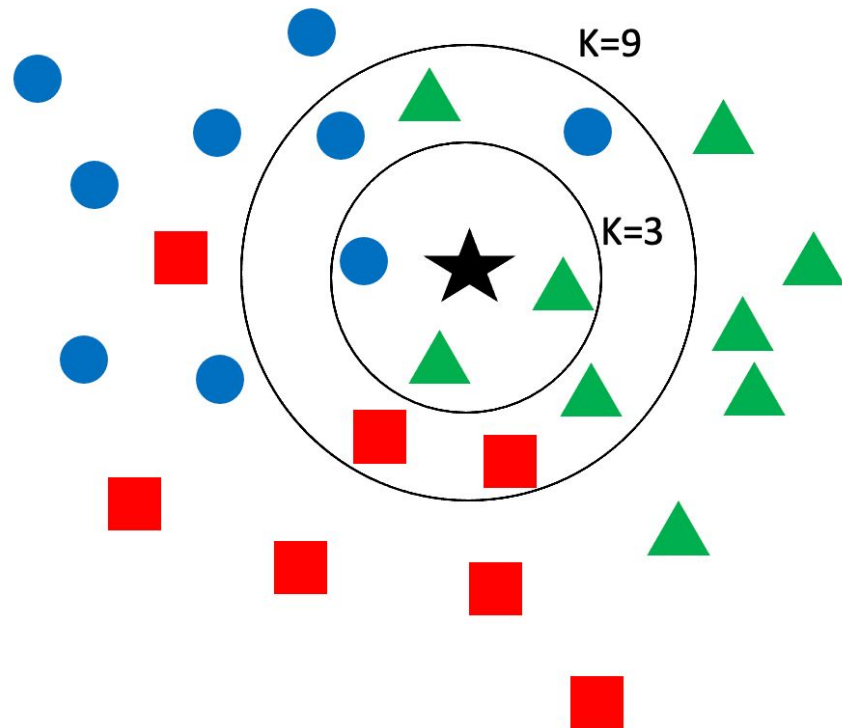


Price
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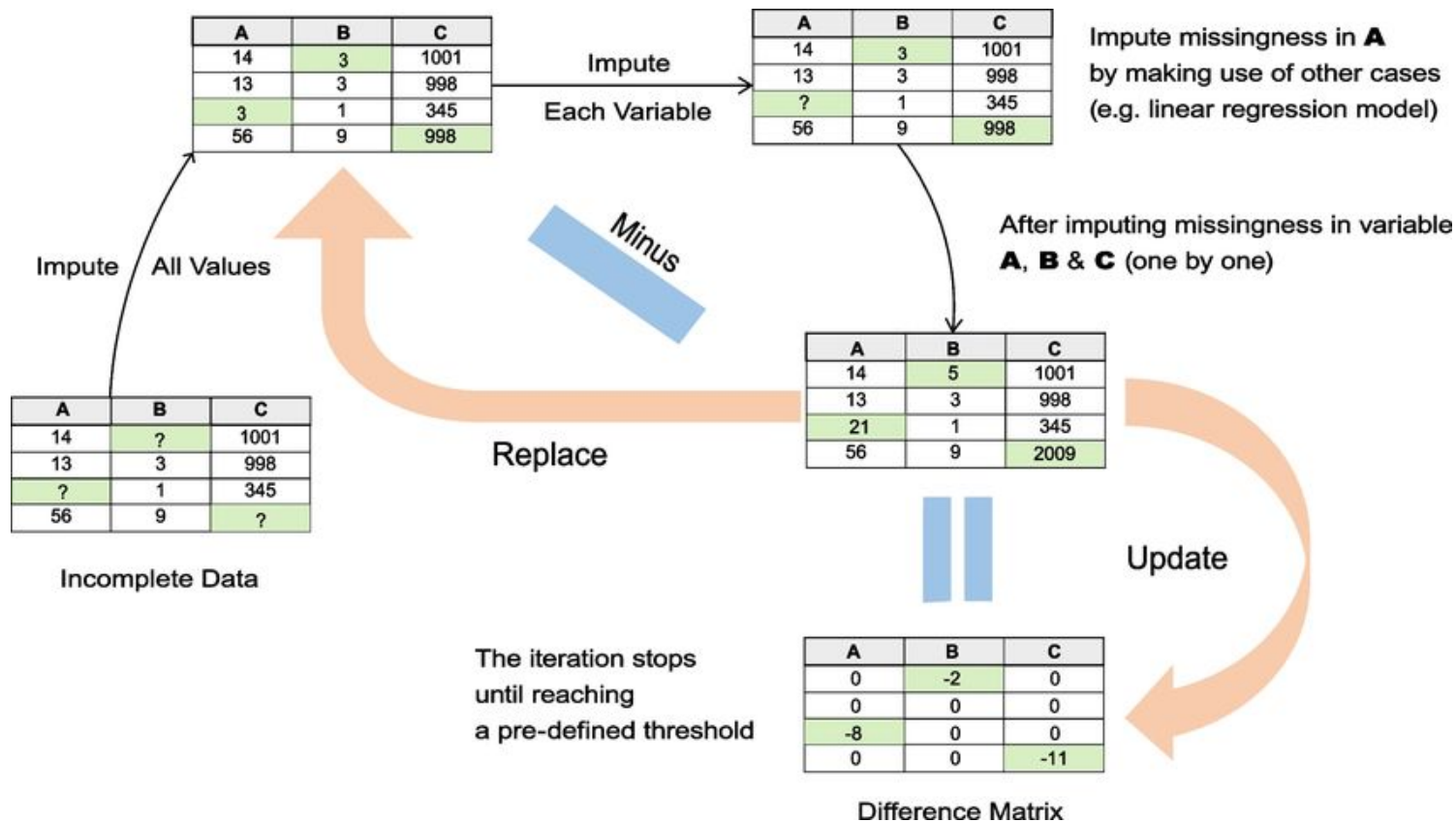
## Module 1: Imputation

- Identification of Neighbours
- Selection of k-neighbours
- Missing values estimation
- Repetition for All Samples



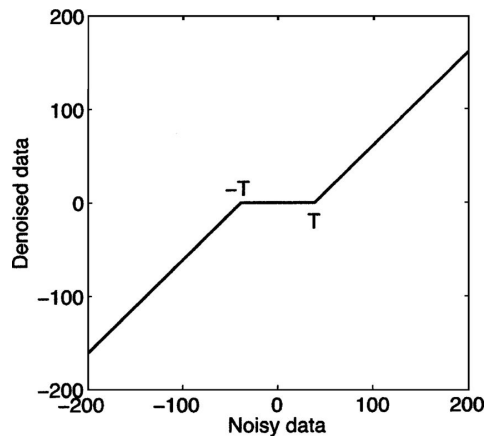
# Imputation

## Multivariate Imputation by Chained Equations (MICE)



# Imputation *SoftImpute* (Singular Value Decomposition)

- Matrix Decomposition
- Dimensional Reduction
- Regularization
- Imputation
- Iterate Process



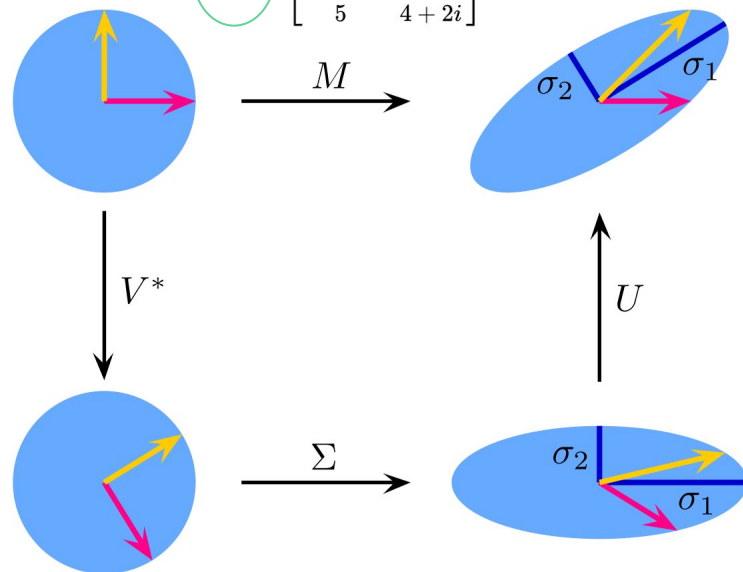
$$\mathbf{A} = \begin{bmatrix} 1 & -2-i & 5 \\ 1+i & i & 4-2i \end{bmatrix}$$

We first transpose the matrix:

$$\mathbf{A}^T = \begin{bmatrix} 1 & 1+i \\ -2-i & i \\ 5 & 4-2i \end{bmatrix}$$

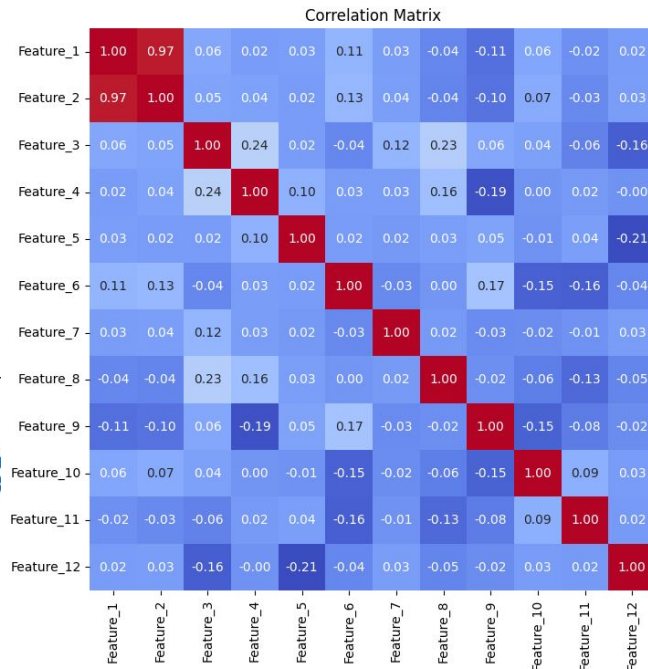
Then we conjugate every entry of the matrix:

$$\mathbf{A}^H = \begin{bmatrix} 1 & 1-i \\ -2+i & -i \\ 5 & 4+2i \end{bmatrix}$$



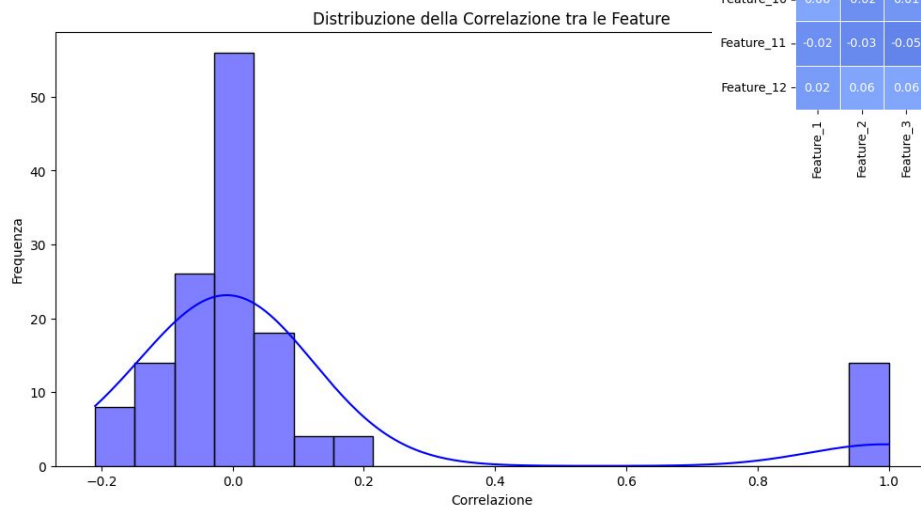
$$M = U \cdot \Sigma \cdot V^*$$





# Module 1: Data Correlation

- Feature Selection
- *Multicollinearity Prevention*
- Feature Engineering
- Noise Reduction

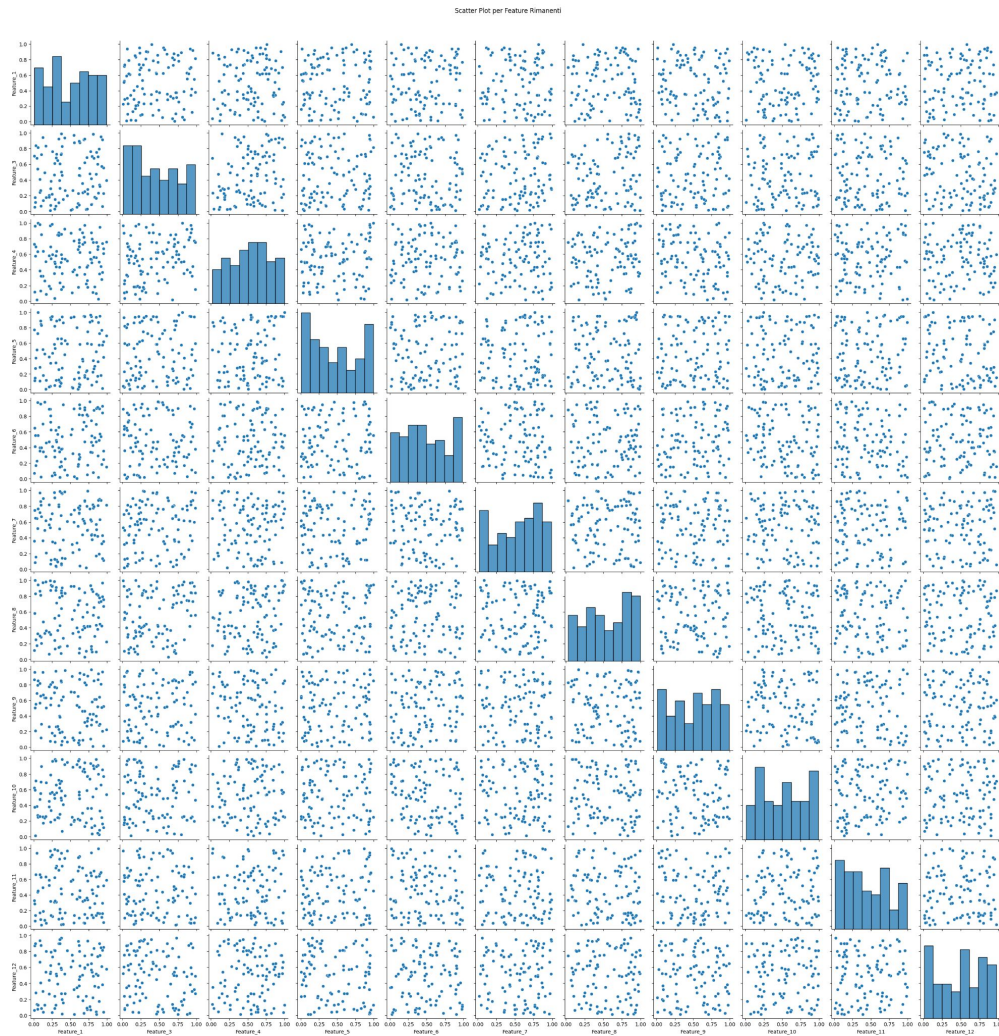


Matrice di Correlazione tra le Feature

Feature_1	1.00	-0.14	-0.10	0.02	0.03	0.11	0.03	-0.04	-0.11	0.06	-0.02	0.02
Feature_2	-0.14	1.00	0.95	-0.10	-0.04	-0.03	-0.10	0.06	0.01	-0.02	-0.03	0.06
Feature_3	-0.10	0.95	1.00	-0.06	-0.05	0.00	-0.08	0.05	0.02	0.01	-0.05	0.06
Feature_4	0.02	-0.10	-0.06	1.00	0.10	0.03	0.03	0.16	-0.19	0.00	0.02	-0.00
Feature_5	0.03	-0.04	-0.05	0.10	1.00	0.02	0.02	0.03	0.05	-0.01	0.04	-0.21
Feature_6	0.11	-0.03	0.00	0.03	0.02	1.00	-0.03	0.00	0.17	-0.15	-0.16	-0.04
Feature_7	0.03	-0.10	-0.08	0.03	0.02	-0.03	1.00	0.02	-0.03	-0.02	-0.01	0.03
Feature_8	-0.04	0.06	0.05	0.16	0.03	0.00	0.02	1.00	-0.02	-0.06	-0.13	-0.05
Feature_9	-0.11	0.01	0.02	-0.19	0.05	0.17	-0.03	-0.02	1.00	-0.15	-0.08	-0.02
Feature_10	0.06	-0.02	0.01	0.00	-0.01	-0.15	-0.02	-0.06	-0.15	1.00	0.09	0.03
Feature_11	-0.02	-0.03	-0.05	0.02	0.04	-0.16	-0.01	-0.13	-0.08	0.09	1.00	0.02
Feature_12	0.02	0.06	0.06	-0.00	-0.21	-0.04	0.03	-0.05	-0.02	0.03	0.02	1.00

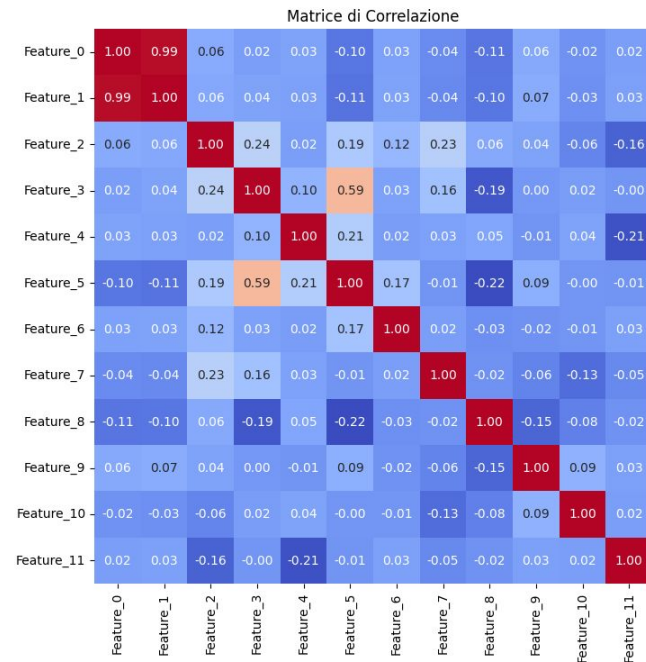
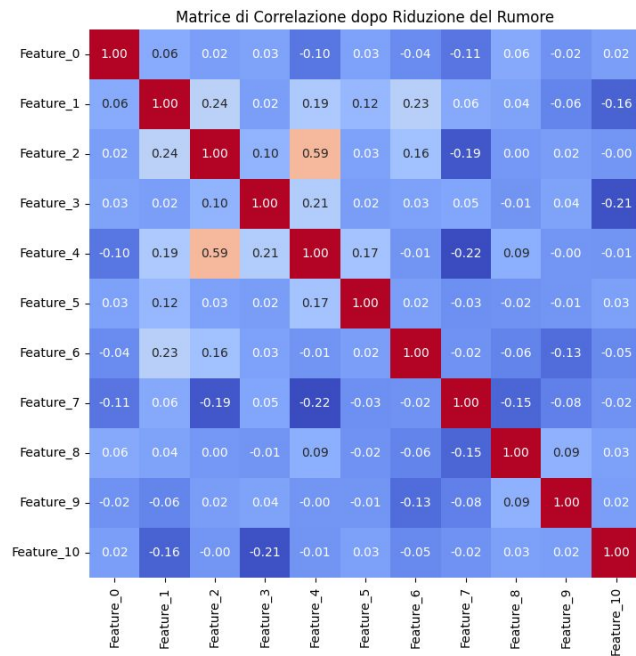
# Module 1: Data Correlation

- Feature Selection
- Multicollinearity Prevention
- *Feature Engineering*
- Noise Reduction



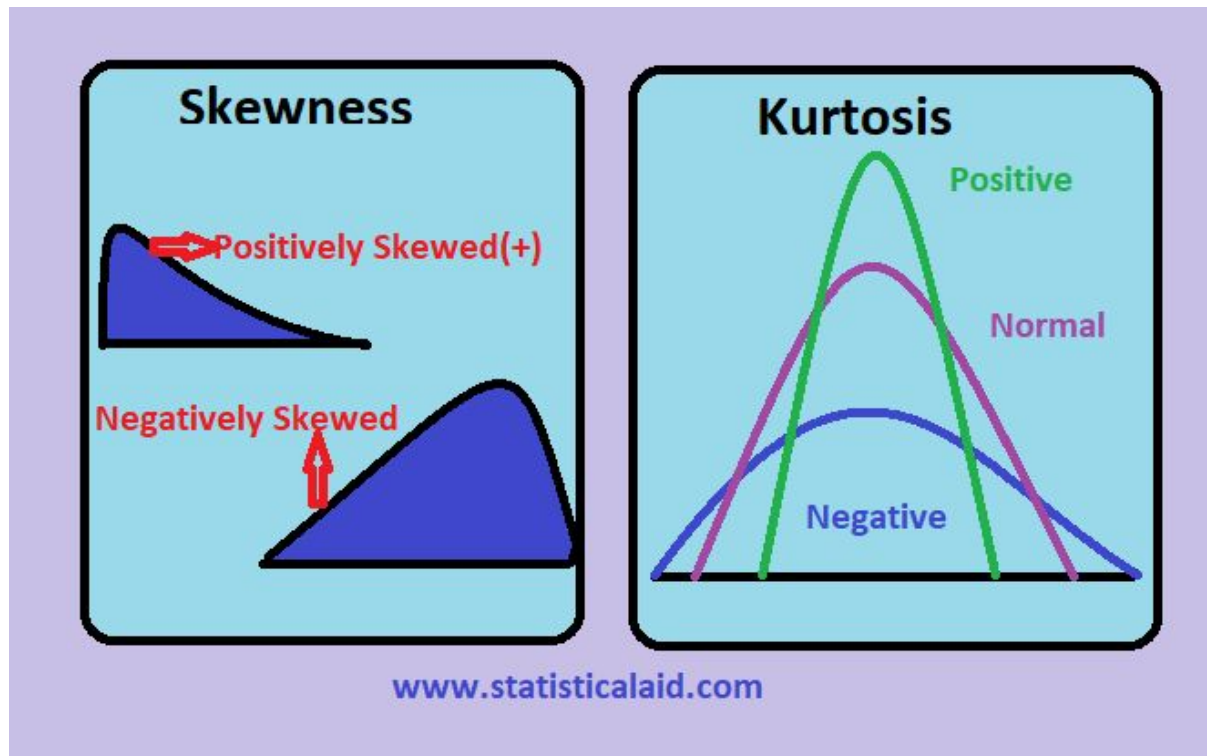
# Module 1: Data Correlation

- Feature Selection
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- Feature Engineering
- *Noise Reduction*



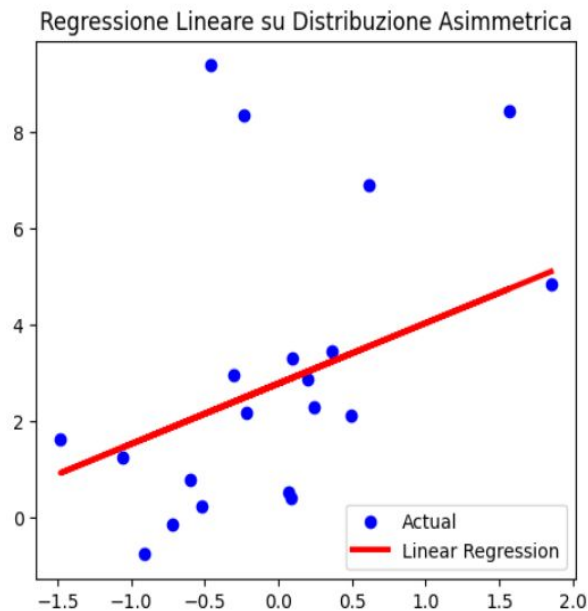
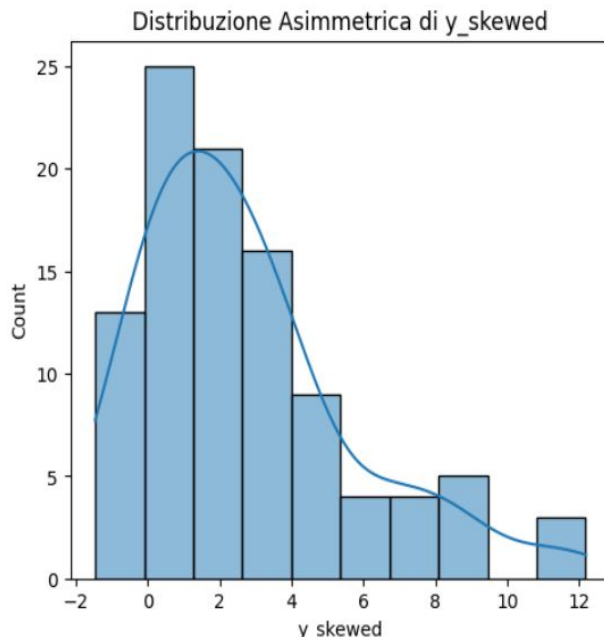
# Module 1: Data Distribution

- Data Information
  - Normal Distribution
  - Skew Distribution
  - Kutosis
- **Multicollinearity**  
**Prevention**
- Feature Engineering
- Noise Reduction



# Module 1: Data Distribution

- Data Information
- Model Choosing
  - linear regression
- Outliers Detection
- Feature Selection

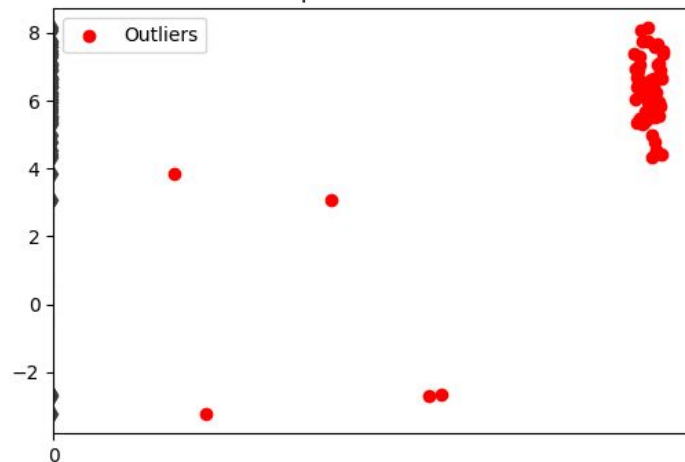




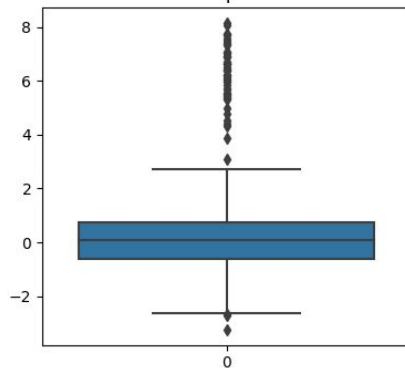
# Module 1: Outliers

- Data Information
- Model Choosing
- Outliers Detection
- Feature Selection

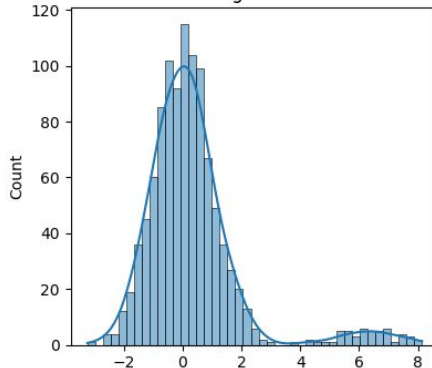
Boxplot con Outliers



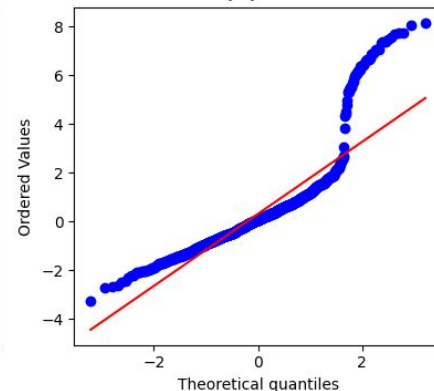
Boxplot



Istogramma

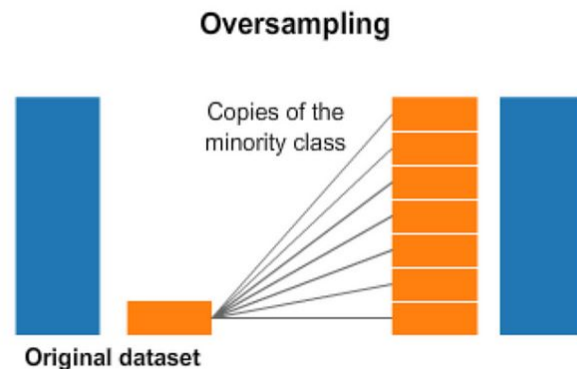
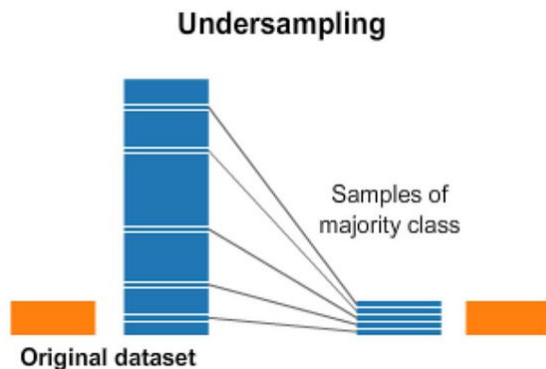
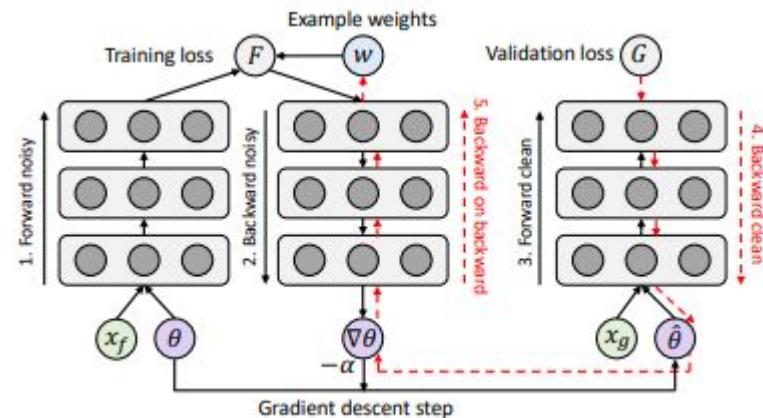


Q-Q Plot



# Module 1: Dataset Balancing

- Reweighting
- Resampling
  - Undersampling
  - oversampling

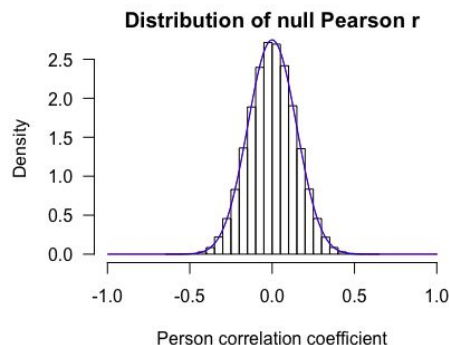




# Module 1: ... *again* Data Correlation

- **Pearson**

- linear correlation
- Normal Distribution
- Linear Scalability
- Without Outliers

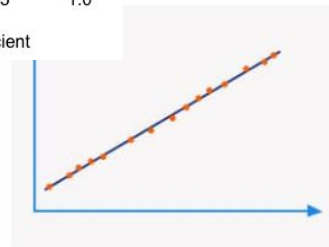


$$r = \frac{N\sum xy - (\sum x)(\sum y)}{\sqrt{[N\sum x^2 - (\sum x)^2][N\sum y^2 - (\sum y)^2]}}$$

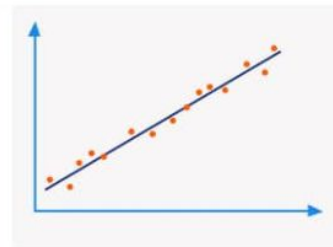
- Spearman

- Kendall

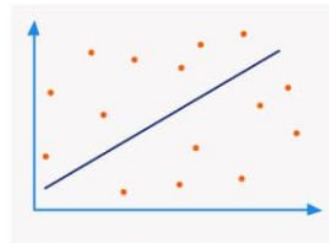
1.  
Large positive  
correlation



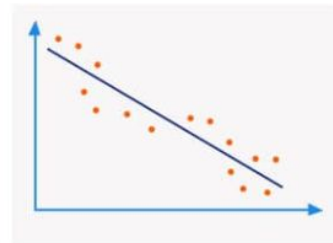
2.  
Medium positive  
correlation



4.  
Weak / no  
correlation

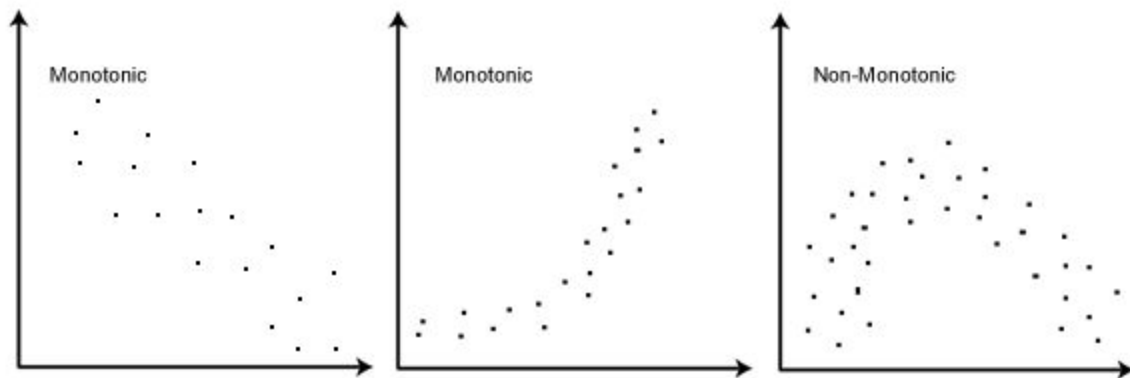
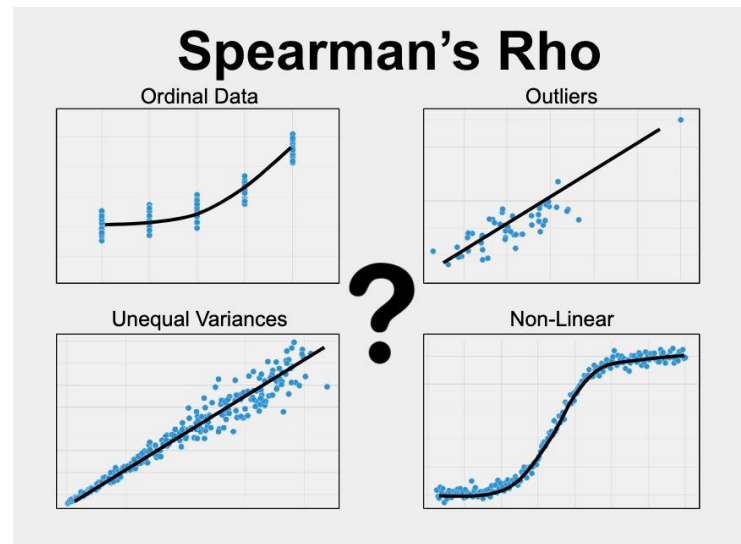


3.  
Small negative  
correlation



# Module 1: ... *again* Data Correlation

- Pearson
- **Spearman**
  - Ordinals
  - Non-linear
  - With Outliers
  - No Normal Distribution
  - Monotone Relation
- Kendall



# Module 1: ... *again* Data Correlation

- Pearson

- Spearman

- **Kendall**

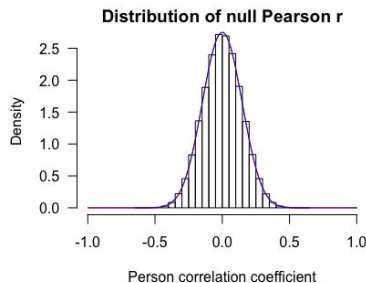
- **Non Normal Distribution**
- **Robustness to Outliers**
- **Ordinal Representation**

$$\tau = \frac{R}{\sqrt{\frac{(n^2 - n - K_x)(n^2 - n - K_y)}{4}}}$$

# Module 1: ... *again* Data Correlation

- **Pearson**

- linear correlation
- Normal Distribution
- Linear Scalability
- Without Outliers

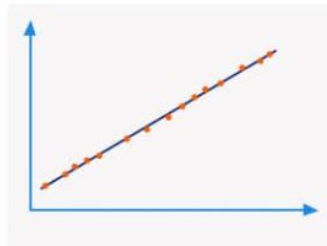


$$r = \frac{N\sum xy - (\sum x)(\sum y)}{\sqrt{[N\sum x^2 - (\sum x)^2][N\sum y^2 - (\sum y)^2]}}$$

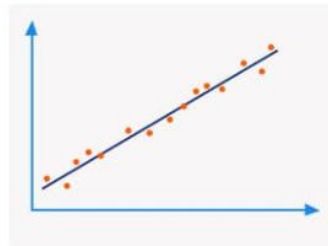
- Spearman

- Kendall

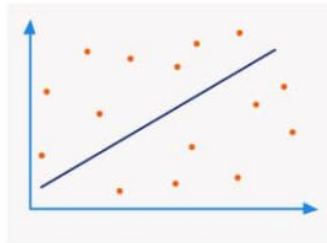
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Large positive  
correlation



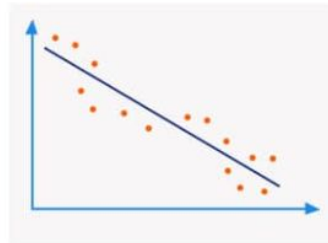
2.  
Medium positive  
correlation



4.  
Weak / no  
correlation

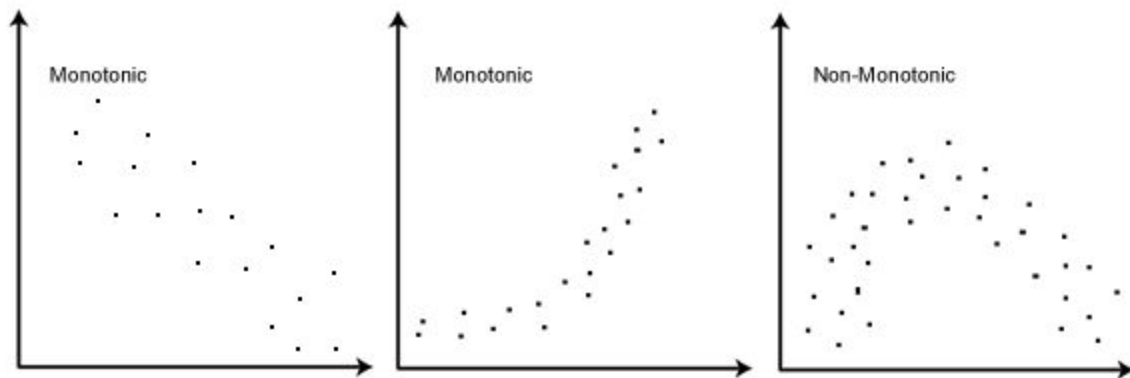
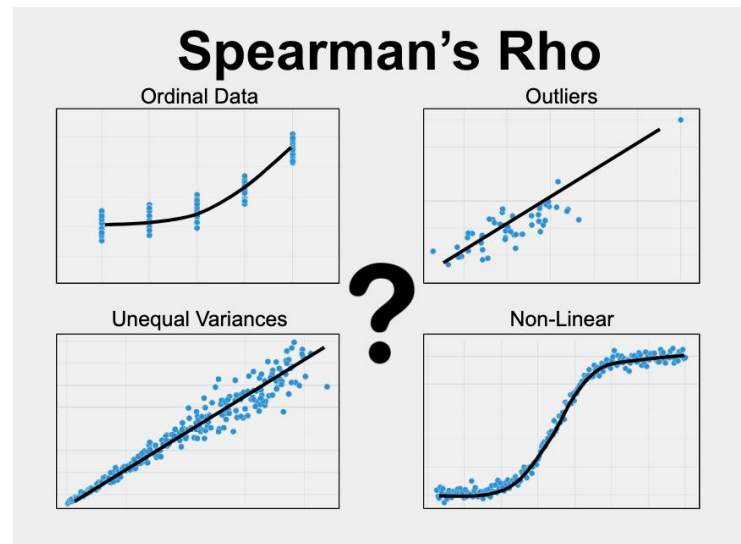


3.  
Small negative  
correlation



# Module 1: ... *again* Data Correlation

- Pearson
- **Spearman**
  - Ordinals
  - Non-linear
  - With Outliers
  - No Normal Distribution
  - Monotone Relation
- Kendall



# Module 1: ... *again* Data Correlation

- Point-Biserial

Mean value of the persons who failed

Mean value of the persons who passed

$$r_{pb} = \frac{\bar{x}_2 - \bar{x}_1}{s_x} \cdot \sqrt{\frac{n_1 \cdot n_2}{n^2}}$$

Number of those who have failed

Number of people who have passed

Total number

- Cramer's V

$$V = \sqrt{\frac{\Phi^2}{\min\{(r-1), (c-1)\}}}$$

- Partial Correlation

$$\rho_{XY|Z} = \frac{N \sum_{i=1}^N e_{X,i} e_{Y,i}}{\sqrt{N \sum_{i=1}^N e_{X,i}^2} \sqrt{N \sum_{i=1}^N e_{Y,i}^2}}$$

- Phi Correlation

- .....

$$MCC = \frac{TN \times TP - FN \times FP}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$

$\rho_{XY|Z}$ : partial correlation of X and Y (controlled for Z)

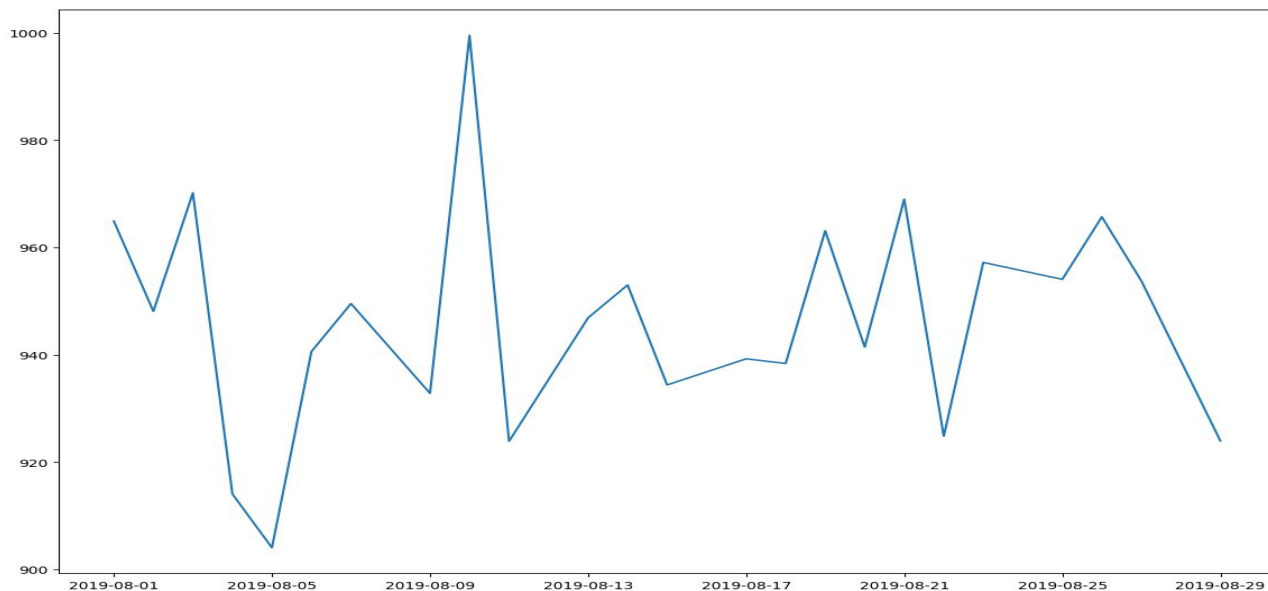
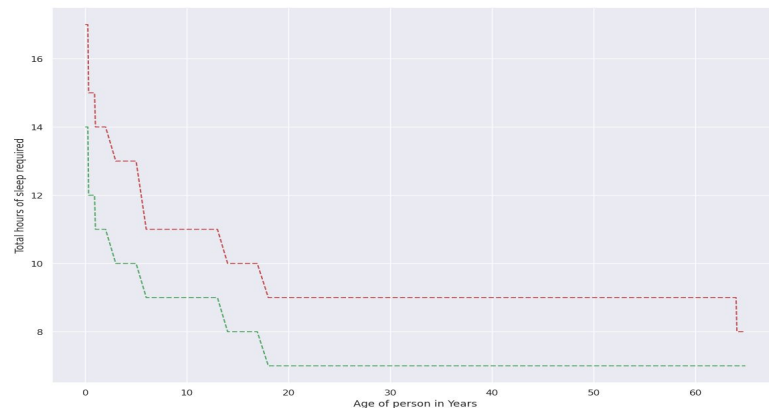
N: number of observations

$e_{X,i}$ : i-th residual of the linear model predicting X by Z

$e_{Y,i}$ : i-th residual of the linear model predicting Y by Z

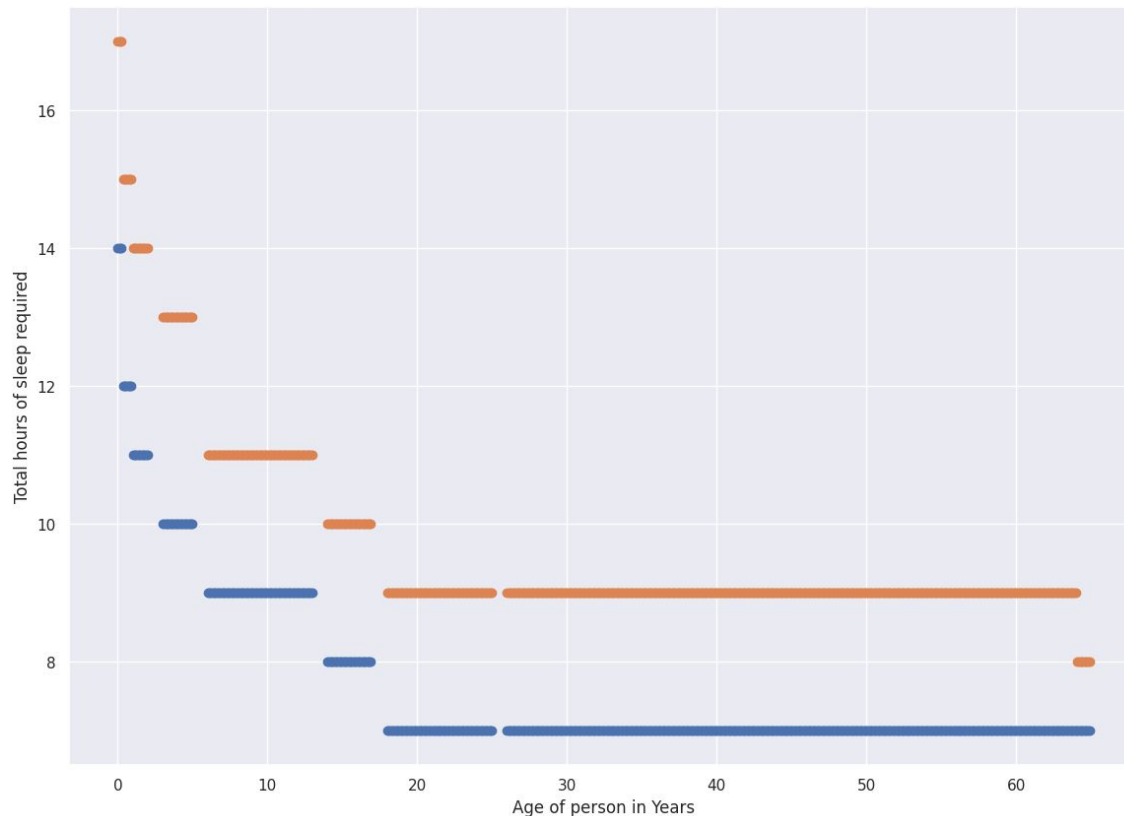
# Module 1: Descriptive Statistics

- Line Chart & Plot
- Scatter Plots
- Area & Stacked Plots
- Pie and Table Charts
- Polar & Lollipop Charts



# Module 1: Descriptive Statistics

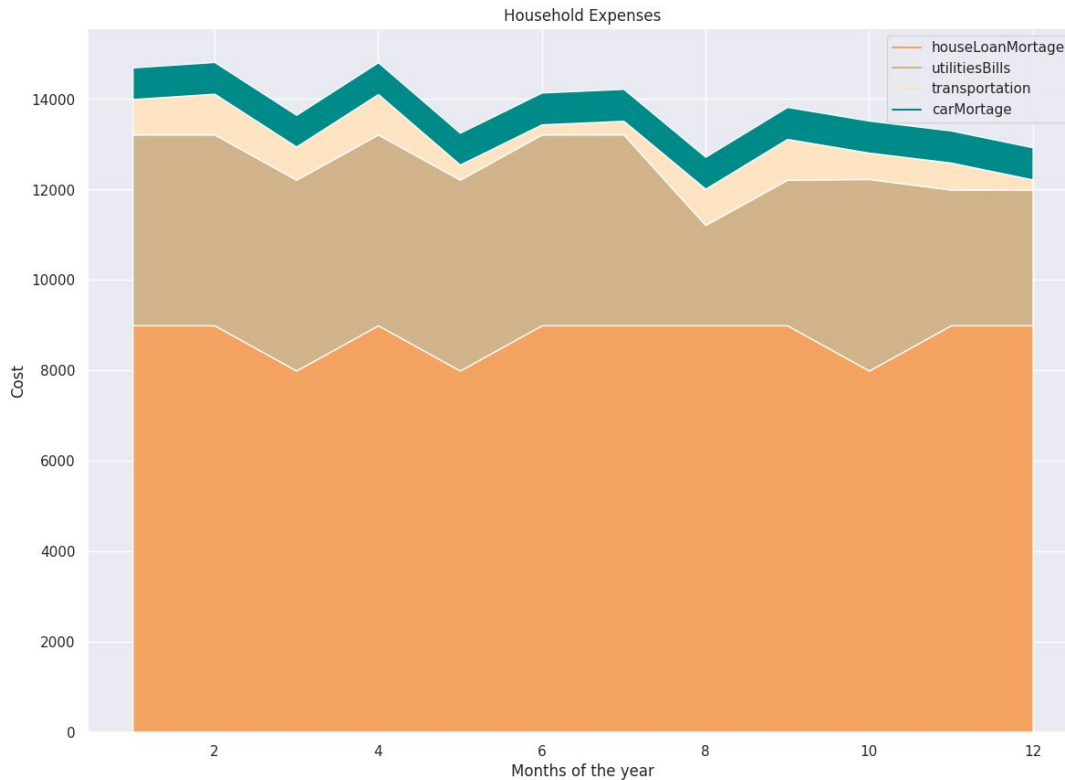
- Line Chart
- **Scatter Plots**
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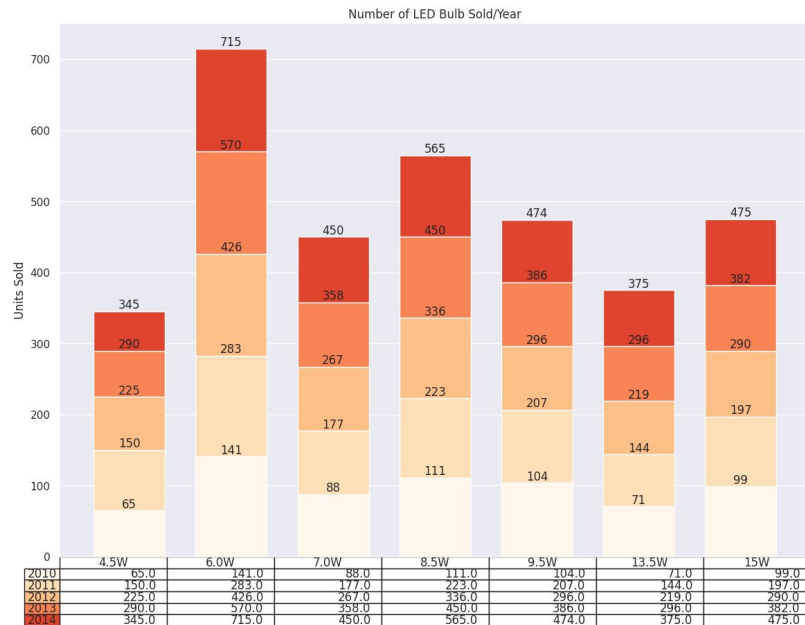
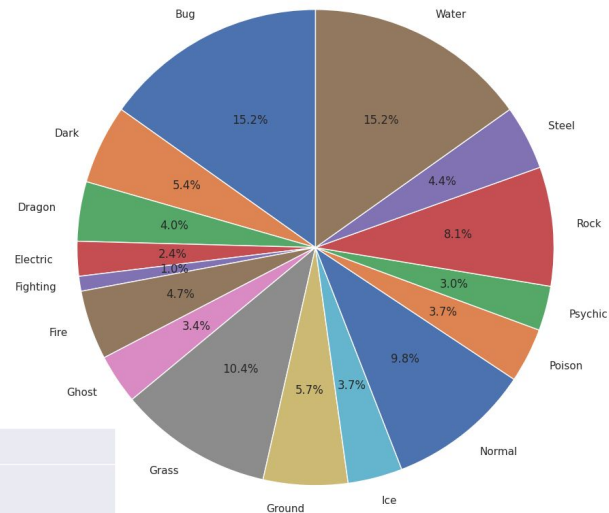
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