Probability and Statistics for Machine Learning

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ML = STATISTICAL learning

- All Machine Learning methods are statistical in nature, since we learn general relationships from a sample/data/observations/measurements

- In order to not just learn "cooking recipes", we will use a minimal mathematical formalism that gives us a uniform and coherent representation of statistical learning

- we have:

  $\Rightarrow$ independent variables x (inputs, features, attributes, explanatory variables)
  $\Rightarrow$ dependent variables y (outputs, responses, explained variables)
  $\Rightarrow$ an unknown relationship, f, that links inputs to outputs, and that we want to learn from the available data
    $\rightarrow$ for predictions
    $\rightarrow$ for inference

Populations and Samples

Definition 1. A population is the set of all objects (observations) being studied. Their number is denoted by N.

Definition 2. A sample is a subset, of size n, $n \leq N$, drawn from the population. We examine these observations to draw conclusions and to make inferences about the population.

For Big Data:

✘ N =ALL ??? No.

✘ Correlation $\Longrightarrow$ Causation ??? No.

Pre-requisite: the mathematical framework

- Suppose we have :

  $\Rightarrow$ a response variable (to explain), Y,
  $\Rightarrow$ p explanatory, variables, $X = (X_1, X_2, \ldots, X_p)$,
  $\Rightarrow$ n samples of data, giving an $(n \times p)$ matrix,

$$X = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & & \\ \vdots & & \ddots & \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

  $\Rightarrow$ a relationship between Y and X of the form

$$Y = f(X) + \epsilon$$

  where
  $\rightarrow$ f is an unknown function of $X_1, X_2, \ldots, X_p$

- $\rightarrow$ ϵ is a random error term, independent of X, and with zero mean

- ML is then an ensemble of approaches for estimating f with the objectsives of
  - $\Rightarrow$ Prediction: $\hat{Y} = \hat{f}(X)$ where $\hat{f}$ is an estimation for f and $\hat{Y}$ is the resulting prediction
  - $\Rightarrow$ Inference: to understand how Y varies as a function of X (correlations, importances, linearity, etc.)

Step 1: Exploratory Data Analysis (EDA)

✔ An initial, critical step of the "data science" process

✔ There are neither hypotheses, nor models - we explore and we try to understand the problem!

✔ The tools of EDA are :

- summary statistics
- basic plots
- graphics

✔ The methodology :

- systematic passage over all the data
- plot all distributions of all the variables ("box plots")
- plot all the time series
- try changes of variables (usually logs or powers)
- look at all the relations two-by-two ("scatterplots")

- calculate all the summary statistics: mean, minumum, maximum, quartiles, outliers

SUMMARY Statistics

- measures of
  - ⇒ central tendancy
  - ⇒ dispersion around the centre

Measures of Central Tendancy

- mean:
$$\bar{x}_j = \frac{1}{n}\sum_{i=1}^{m} x_{ij}, \quad j = 1, \ldots, p$$

```
> Xj    = c(1,2,3,4,5)
> Xbarj = mean(Xj)
```

- median: value for which at most the half of the population is less than, and at least half is greater than,

$$\mathrm{median}(x) = \begin{cases} x_{(n+1)/2}, & \text{if } n \text{ odd} \\ \dfrac{x_{(n/2)} + x_{(n/2)+1}}{2}, & \text{if } n \text{ even} \end{cases}$$

```
> Xmedj = median(Xj)
```

- mode: the most frequent value (for which the frequency/probability is maximal)

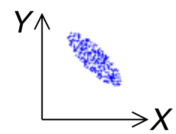
Measures of Dispersion

- variance and standard deviation:

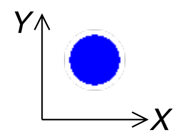
$$s^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

```
> Xvar = var(Xj)
> Xstd = sd(Xj)
```

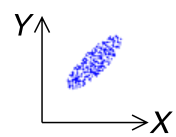
- covariance between k variables, with n observations each, is a $k \times k$ matrix with elements



cov(X,Y)<0



cov(X,Y)≈0



cov(X,Y)>0

$$q_{jk} = \frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)$$

```
> Xcov = cov(XX) # covariance
> Xcor = cor(XX) # correlation, entre -1 et 1
```

- quartiles, quantiles and inter-quartile distance: z is the k-th q-quantile, if

$$\Pr\left[X < z\right] \leq \frac{k}{q}$$

$\Rightarrow$ the median is the second quartile, Q_2

$\Rightarrow$ la inter-quartile distance

$$\mathrm{IQR} = Q_3 - Q_1$$

is a measure of dispersion

$\Rightarrow$ the 100-quantiles are called percentiles

```
> range(Xj) # max - min
> quantile(Xj) #  0, 25, 50, 75 et 100%
> IQR(Xj)
```

Summary Statistics

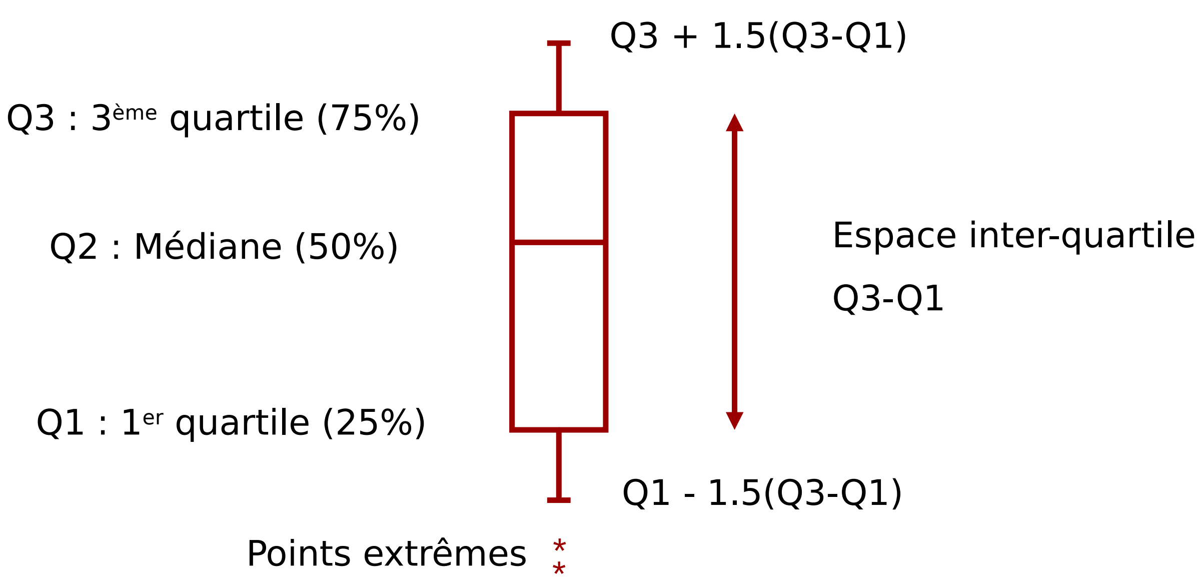
- the 5-number summary of Tukey is employed systematically for any data analysis

  1. minimum
  2. first quartile
  3. median
  4. third quartile
  5. maximum

```
> fivenum(Xj)
> summary(XX)
```

Plots and Graphics for EDA

- box-plots:

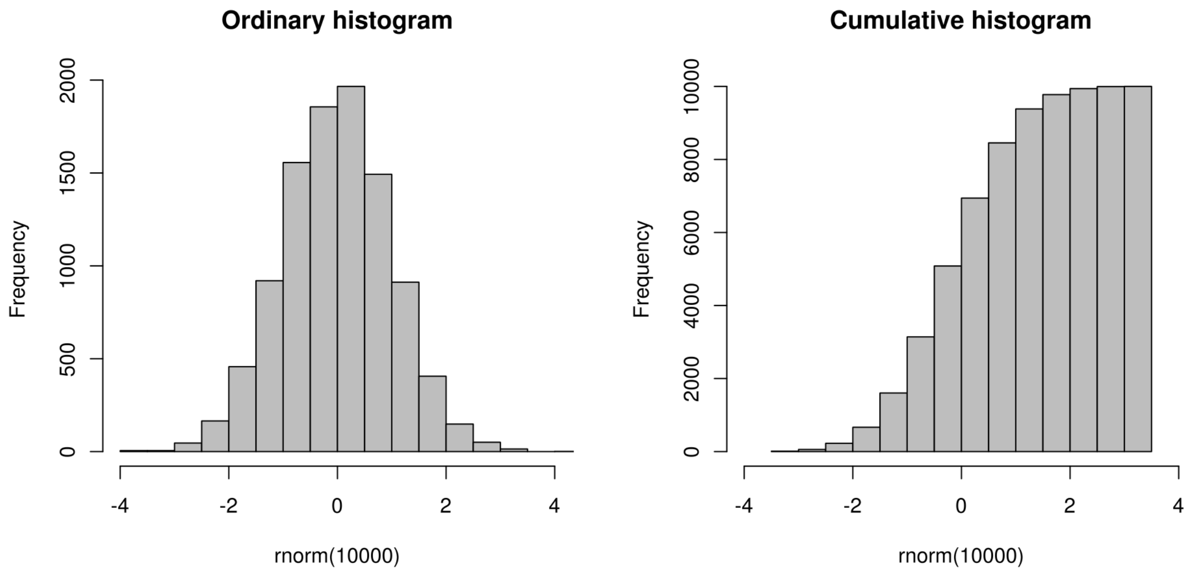


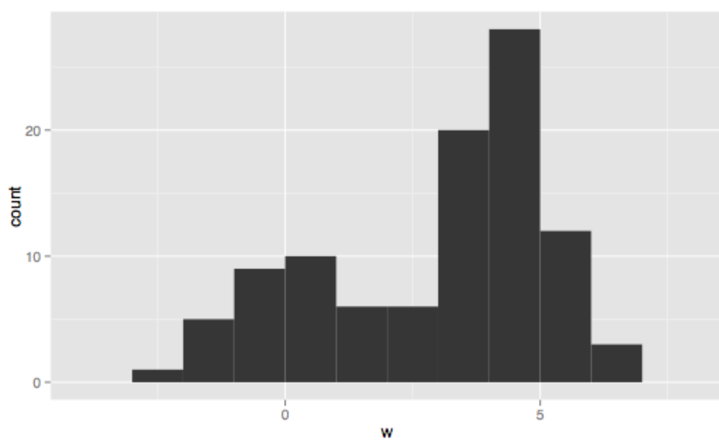

```
> boxplot(Xj)
```

- histograms:

$\Rightarrow$ approximates the probability density function
$\Rightarrow$ allows to detecti multi-modality...

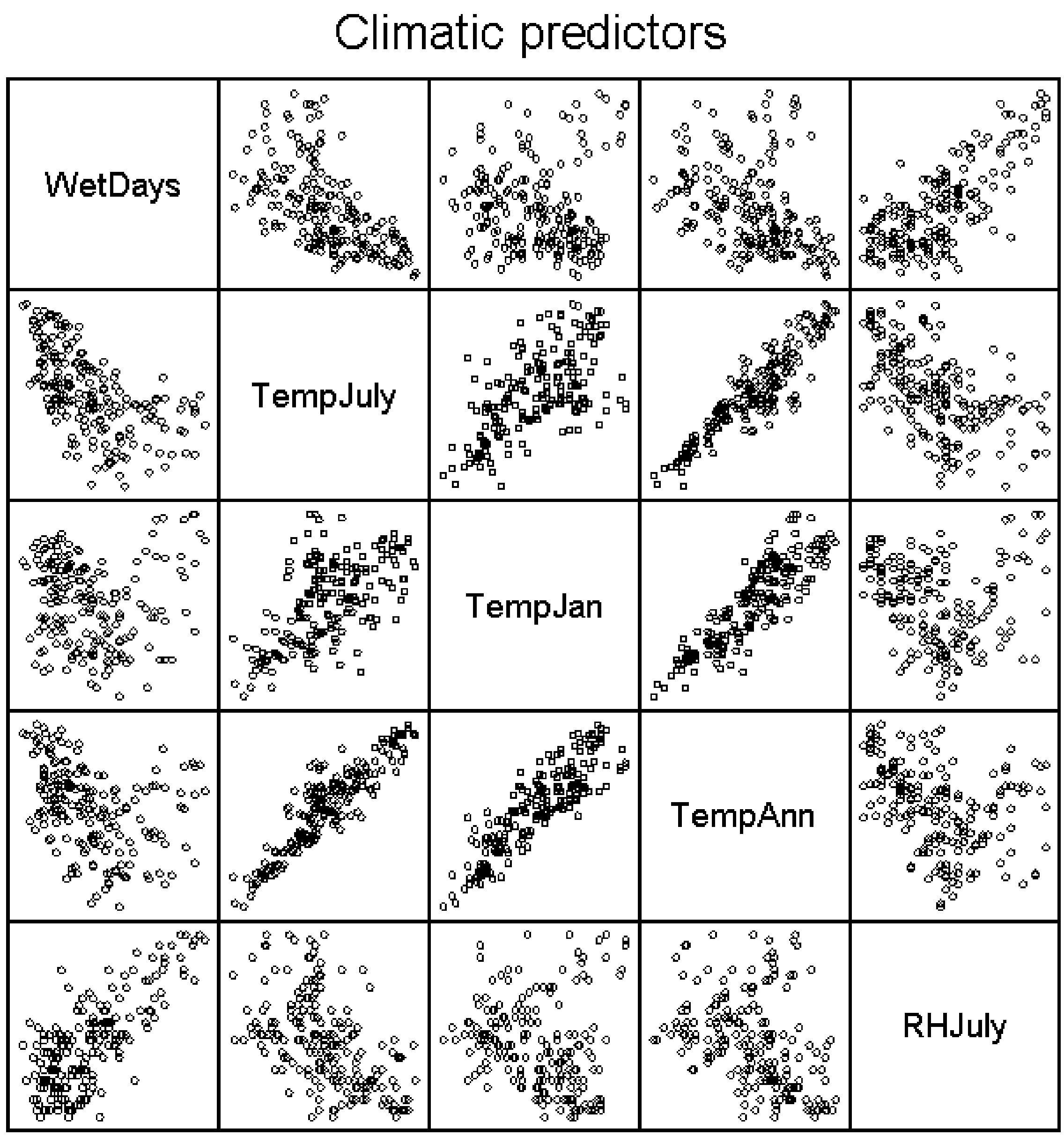
```
> hist(Xj)
```





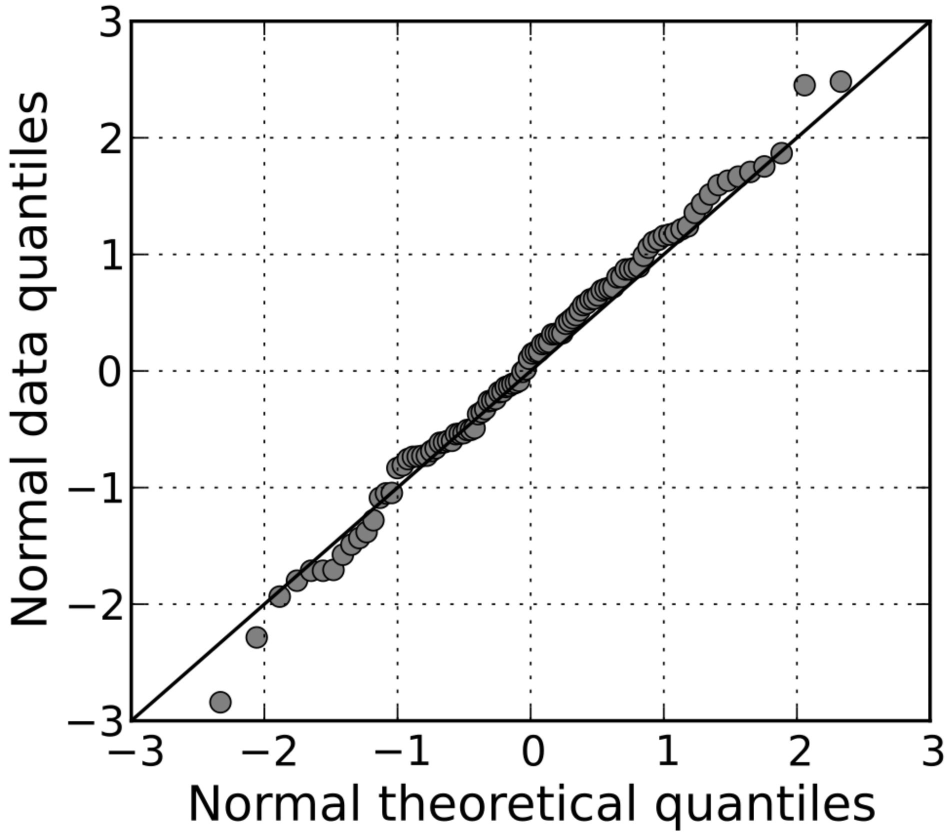
- scatter-plots: in the multi-variable case, allows to display all the correlations, 2-by-2

```
> plot(XX)
```



- q-q plots: graphic of quantiles to verify the hypothese of normality (Gaussian)

```
> qqnorm(Xj); qqline(Xj)
```



Significance and Covariates

- the 2 fundamental notions for UNDERSTANDING any statistical model
  - ⇒ significance (bad!) and confidence intervals (better)
  - ⇒ covariates need to be chosen judiciously (can produce false significance)

Significance Tests

Example. Compare a new and an old treatment against hypertension.

- suppose the data **seem** to indicate that the new treatment is better

- can we exclude a sampling «accident», where the new treatment was given almost exclusively to subjects in good health???

- the significance test would state that this result is very unlikely (small value of p) under the null hypothesis (= no effect)

- Conclusion (dangerous!): the two treatments have a significant diffference at level α ($> p$).

Significance Tests : conclusion

- significance tests should be avoided (official recommendation of the ASA in 2016)
  - $\Rightarrow$ at worst, they are misleading
  - $\Rightarrow$ at best, they are uninformative
- producing a confidence interval (point estimate +/- error margin) is much better
  - $\Rightarrow$ usually, at a 95% level
  - $\Rightarrow$ "in 95% of all possible samples, the empirical estimate will lie within the error margin of the true value of the population"
  - $\Rightarrow$ however, we will not repeat the sampling numerous times—this is ususally impossible... hence the interest of Bayesian approaches... (TBC)

Explanatory Variables

- we study the relationship between a variable Y and a variable X

Example. Evaluation in 4 hospitals of survival rates after a heart attack

- let the response $Y = 1$ if the patient survives, $Y = 0$ if not.

- let $X = 1, \ldots, 4$ be the identifier of the hospital

- measuring the relationship between Y and X implies here to compare the 4 hospitals in terms of the survival rate...

  $\Rightarrow$ but 1 of the 4 hospitals serves a zone with a large proportion of old patients
  $\Rightarrow$ so a direct comparison would be unfair, and inexact...

- we need to introduce a new explanatory variable , $Z = \text{age}$ and measure the relationship between Y and X keeping Z constant (or by age intervals)

- a correlation can pass from positive to negative (change of sign) once the covariate Z is taken into account

$\Rightarrow$ Simpson's paradox..
$\Rightarrow$ related to causality! (TBC)

Cross Validation

- an ensemble of techniques for testing the predictive power of a statistical learning model

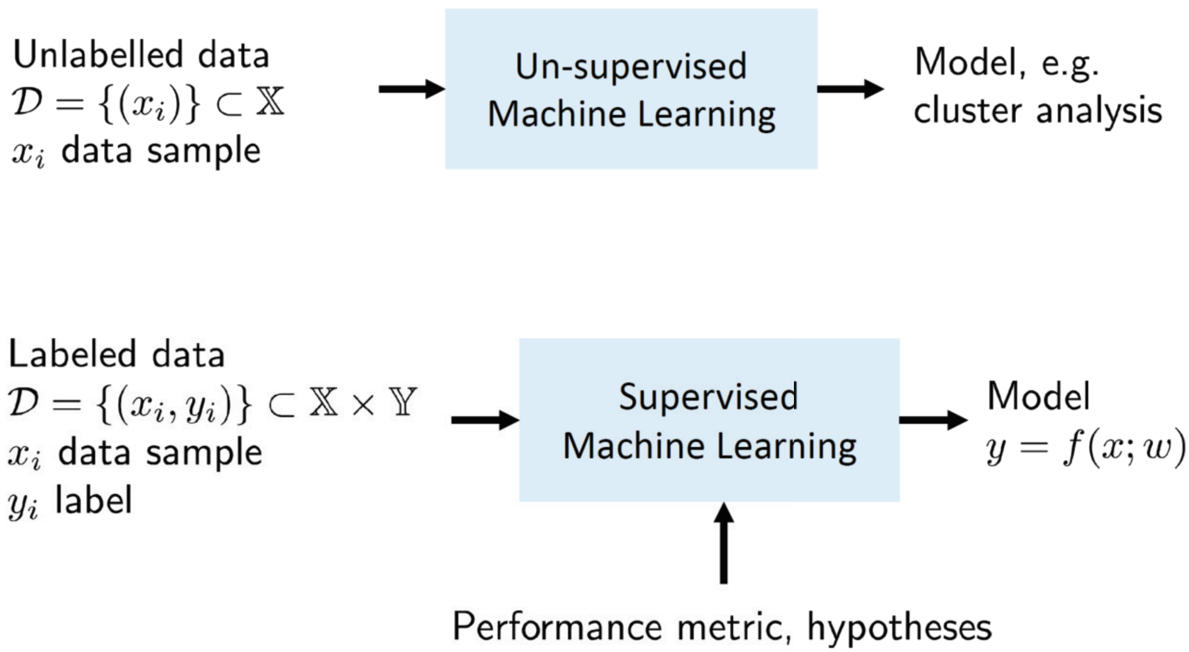
- indispensable step for validating the robustness of a model

  $\Rightarrow$ avoids the "good luck" effect

- also possible to propose confidence intervals

  $\Rightarrow$ using the "bootstrap"

ML Frameworks: Supervised and Unsupervised



ML Frameworks: Regression and Classification

Variables can be characterized as:

- ✔ quantitative, taking on numerical values
- ✔ qualitative (or categorical), that take values in one of K different classes (or categories).

The problems are then of type:

- ✔ regression when we have quantitative variables,
- ✔ classification for qualitative variables.

Labeled data
$\mathcal{D} = \{(x_i, y_i)\} \subset \mathbb{X} \times \mathbb{Y}$
$x_i \in \mathcal{D}_x$ data samples
$y_i \in \mathcal{D}_y$ labels
$\mathbf{x} = [x_i]$
$\mathbf{y} = [y_i]$

Supervised Machine Learning

Model
$y = f(x; w)$

Performance metric, hypothesis on f

Model purpose – Regression

- The model f shall map $x \mapsto y$ and approximate an unknown function $\hat{f} : \mathbb{X} \to \mathbb{Y}$
- $y_i \in \mathbb{Y} \subseteq \mathbb{R}^{n_y}$
- Examples: data-driven modeling, energy forecasting, ...

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Supervised Machine Learning

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Model purpose – Classification

- The model f shall map $x \mapsto y$ and approximate an unknown function $\hat{f} : \mathbb{X} \to \mathbb{Y}$
- $y_i \in \mathbb{Y} \subseteq \mathbb{N}^{n_y}$
- Examples: spam filter, fraud detection, fault detection, ...

- the only difference is the space in which y_i takes its values:

$\Rightarrow$ continuous space, $\mathbb{R}^n$, for regression
$\Rightarrow$ discrete space, $\mathbb{N}^n$, for classification

Recall: Which model for which task?

Class	Model	Task
Supervised	linear regression	R
	CART (trees)	R&C
	SVM	R&C
	NN	R&C
	k-NN	C
	Naive Bayes	C
Unsupervised	k-means	Clustering
	dendrogram	Clustering
	PCA	pattern

R = regression, C = classification