# Machine Learning

## What is machine learning?

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(1) `Data availability`: huge growth due to automation, digitalization, web applications.

(2) `Computing power`: significant increase thanks to GPU computing, parallelization, etc.

(3) `The learning algorithms`: theoretical developments of new statistical models and training methods.

# The statistical framework

Types of variables:

- quantitative variables take values in an ordered set, typically the real numbers $\mathbb{R}$;
- qualitative variables (also called categorical or factor) take values in a finite set $\mathcal{G} = \{\mathcal{G}_1, \dots, \mathcal{G}_q\}$ without ordering, e.g., $\{$Yes, No$\}$, $\{$blue, red, green, yellow$\}$, etc.

Supervised learning

- We observe training data $(x_i, y_i)$, $i = 1, \dots, n$ where
  - the inputs $x_i \in \mathbb{R}^p$ are called predictors, covariates or features;
  - the outputs $y_i$ are called responses (in this course we assume they are univariate).
- The goal is to predict the (unknown) response $y_0$ for a new (known) predictor $x_0$.
- Regression: the responses $y_i \in \mathbb{R}$ are quantitative.
- Classification: the responses $y_i \in \mathcal{G}$ are qualitative.

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- We observe `training data` $(x_i, y_i)$, $i = 1, \ldots, n$ where
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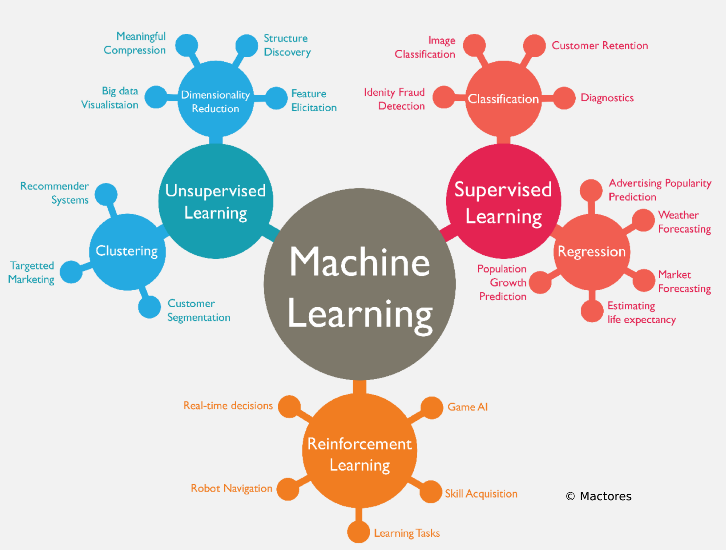
- `Regression`: the responses $y_i \in \mathbb{R}$ are quantitative.
- `Classification`: the responses $y_i \in \mathcal{G}$ are qualitative.

Unsupervised learning

- We only observe multivariate data $x_i \in \mathbb{R}^p$, $i = 1, \ldots, n$ but without a particular response.
- The goal is to `summarize`, `understand`, `interpret` and `visualize` the data.

# Machine Learning: an overview



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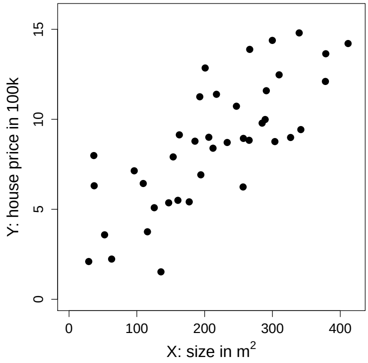

# Regression: simple linear model

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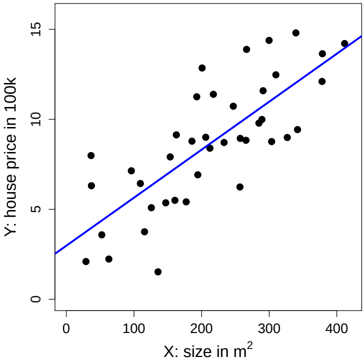


- Linear regression

$$\widehat{y}_0 = \widehat{\beta}_0 + \widehat{\beta}_1 x_0$$

- The numbers $\widehat{\beta}_0, \widehat{\beta}_1 \in \mathbb{R}$ are estimated model parameters.

# Regression: the kNN method

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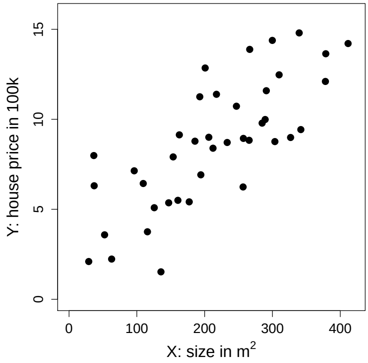


- The k-Nearest-Neighbor (kNN) method

$$\widehat{y}_0 = \frac{1}{k} \sum_{i: x_i \in N_k(x_0)} y_i$$
$$= \mathrm{ave}\{y_i : x_i \in N_k(x_0)\},$$

$N_k(x_0)$ are the $k$ closest points $x_i$ to $x_0$.
- The number $k$ is a tuning parameter.

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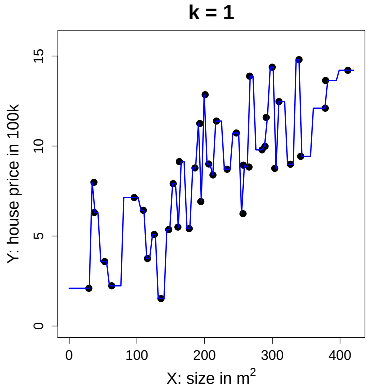


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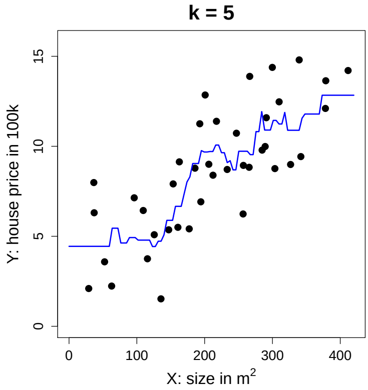


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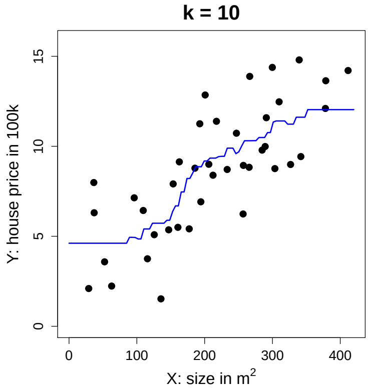


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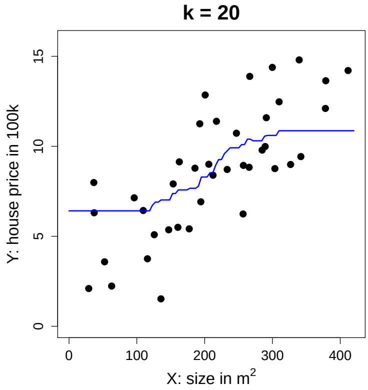


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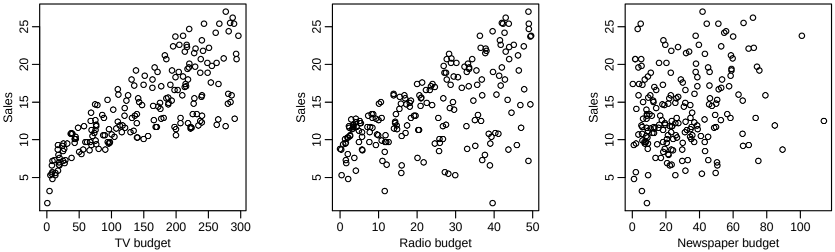
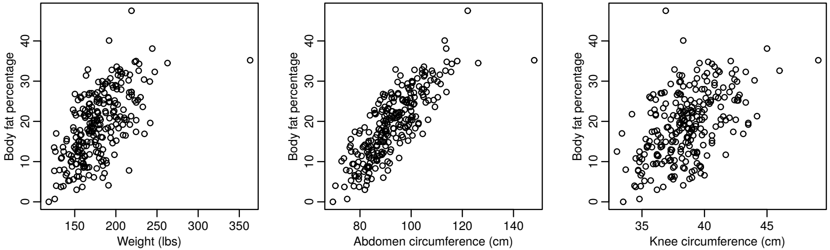
The `Advertising` data set contains `sales`, in thousands of units, as a function of `TV`, `radio`, and `newspaper` budgets, in thousands of dollars, for 200 different markets.



# Medical application: body fat

Data set bodyfat (R library mfp). The data set contains body fat estimates (siri) for 252 men with measurements of different body attributes. The first 10 measurements and a plot of the responses versus some of the predictors:

| siri | age | weight | height | neck | chest | abdo | hip | thigh | knee | ankle | biceps | forearm | wrist |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 12.3 | 23 | 154.25 | 67.75 | 36.2 | 93.1 | 85.2 | 94.5 | 59.0 | 37.3 | 21.9 | 32.0 | 27.4 | 17.1 |
| 6.1 | 22 | 173.25 | 72.25 | 38.5 | 93.6 | 83.0 | 98.7 | 58.7 | 37.3 | 23.4 | 30.5 | 28.9 | 18.2 |
| 25.3 | 22 | 154.00 | 66.25 | 34.0 | 95.8 | 87.9 | 99.2 | 59.6 | 38.9 | 24.0 | 28.8 | 25.2 | 16.6 |
| 10.4 | 26 | 184.75 | 72.25 | 37.4 | 101.8 | 86.4 | 101.2 | 60.1 | 37.3 | 22.8 | 32.4 | 29.4 | 18.2 |
| 28.7 | 24 | 184.25 | 71.25 | 34.4 | 97.3 | 100.0 | 101.9 | 63.2 | 42.2 | 24.0 | 32.2 | 27.7 | 17.7 |
| 20.9 | 24 | 210.25 | 74.75 | 39.0 | 104.5 | 94.4 | 107.8 | 66.0 | 42.0 | 25.6 | 35.7 | 30.6 | 18.8 |
| 19.2 | 26 | 181.00 | 69.75 | 36.4 | 105.1 | 90.7 | 100.3 | 58.4 | 38.3 | 22.9 | 31.9 | 27.8 | 17.7 |
| 12.4 | 25 | 176.00 | 72.50 | 37.8 | 99.6 | 88.5 | 97.1 | 60.0 | 39.4 | 23.2 | 30.5 | 29.0 | 18.8 |
| 4.1 | 25 | 191.00 | 74.00 | 38.1 | 100.9 | 82.5 | 99.9 | 62.9 | 38.3 | 23.8 | 35.9 | 31.1 | 18.2 |
| 11.7 | 23 | 198.25 | 73.50 | 42.1 | 99.6 | 88.6 | 104.1 | 63.1 | 41.7 | 25.0 | 35.6 | 30.0 | 19.2 |



# Classification: simple linear regression

**Data:** Observations $(x_1, y_1), \ldots, (x_n, y_n)$, where $y_i \in \mathcal{G} = \{0, 1\}$
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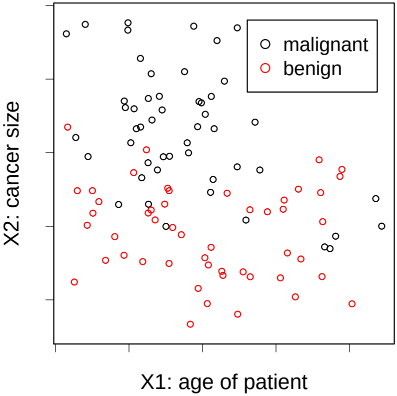

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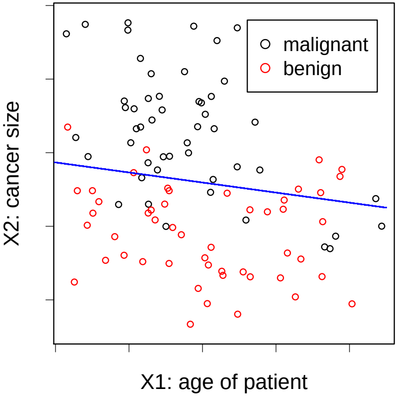


- Directly apply `linear regression` treating the classes as quantitative values 0 and 1. The prediction is

$$\widehat{y}_0 = \begin{cases} 1, & \text{if } \widehat{\beta}_0 + \widehat{\beta}^T x_0 \geq 1/2, \\ 0, & \text{otherwise.} \end{cases}$$

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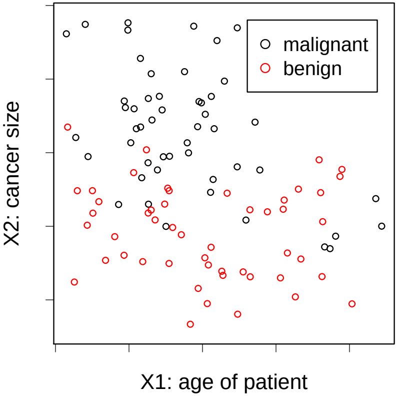


- The k-Nearest-Neighbor (kNN) method predicts the majority of classes in the neighborhood

$$\widehat{y}_0 = \begin{cases} 1, & \text{if } \frac{1}{k} \sum_{i: x_i \in N_k(x_0)} \mathbf{1}\{y_i = 1\} > 1/2, \\ 0, & \text{otherwise.} \end{cases}$$

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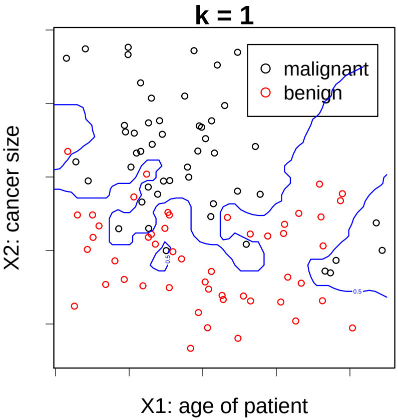


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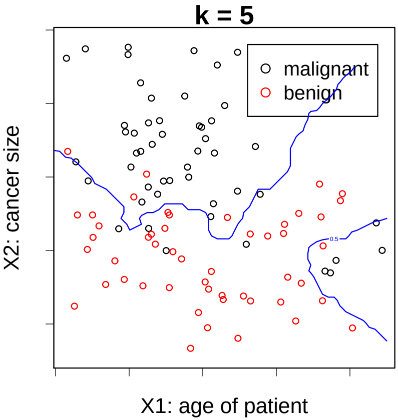


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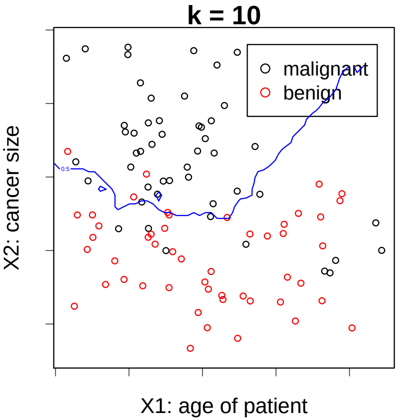


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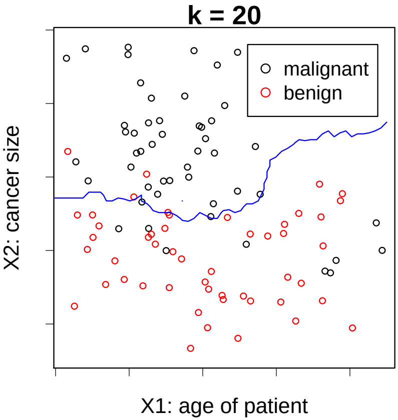


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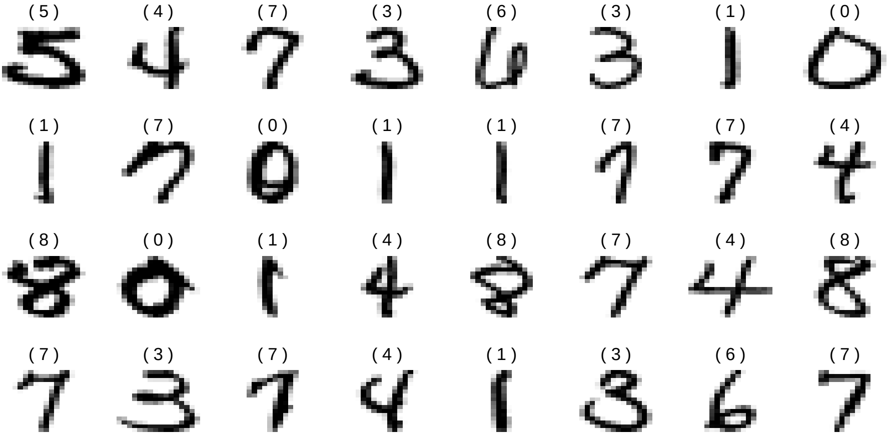
# Example: spam classification

The spam data set (R library kernlab). 4601 emails classified as one of two classes, i.e., $G \in \{\texttt{spam, nonspam}\}$, based on and 57 predictors indicating the frequency of certain words and characters in the e-mail. A subset of the data:

| | type | george | free | credit | money | hp | business | your | ! | capitalTotal |
|---|---|---|---|---|---|---|---|---|---|---|
| 1222 | spam | 0.00 | 0.00 | 5.19 | 0.64 | 0.00 | 1.29 | 1.29 | 0.09 | 135.00 |
| 1712 | spam | 0.00 | 0.44 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 186.00 |
| 2635 | nonspam | 0.66 | 1.33 | 0.00 | 0.22 | 3.34 | 0.00 | 0.44 | 0.37 | 411.00 |
| 4176 | nonspam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.22 | 0.04 | 97.00 |
| 928 | spam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.40 | 495.00 |
| 4129 | nonspam | 0.00 | 0.00 | 0.00 | 1.16 | 0.00 | 0.00 | 1.16 | 0.49 | 34.00 |
| 4341 | nonspam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.77 | 18.00 |
| 3036 | nonspam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 2.32 | 0.00 | 37.00 |
| 2890 | nonspam | 0.00 | 0.00 | 0.00 | 0.00 | 1.72 | 0.00 | 2.58 | 0.11 | 58.00 |
| 284 | spam | 0.00 | 0.40 | 1.81 | 0.60 | 0.00 | 1.61 | 2.62 | 1.45 | 513.00 |
| 946 | spam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.03 | 339.00 |
| 811 | spam | 0.00 | 0.00 | 1.02 | 0.00 | 0.34 | 0.00 | 0.68 | 0.90 | 1330.00 |
| 3153 | nonspam | 0.38 | 0.00 | 0.00 | 0.00 | 0.90 | 0.00 | 0.00 | 0.00 | 1232.00 |
| 1763 | spam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 11.11 | 0.00 | 4.00 |
| 3532 | nonspam | 2.00 | 0.00 | 0.00 | 0.00 | 4.00 | 0.00 | 0.00 | 0.00 | 46.00 |
| 2283 | nonspam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 14.00 |
| 3291 | nonspam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 1.00 |
| 4547 | nonspam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 5.00 |
| 1742 | spam | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.47 | 0.69 | 239.00 |
| 3563 | nonspam | 4.16 | 0.00 | 0.00 | 0.00 | 8.33 | 0.00 | 0.00 | 0.00 | 30.00 |

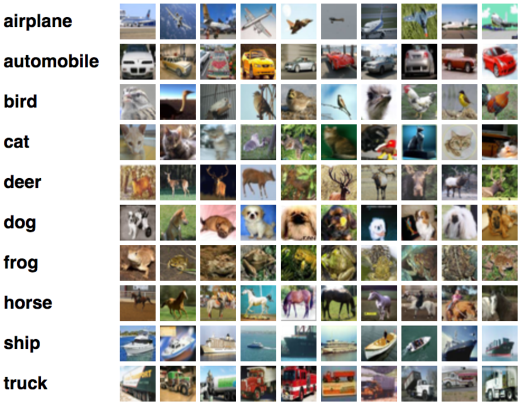
# Example: handwritten characters/digits recognition

Data set from [ESL] homepage: handwritten digits ($16 \times 16$ grey scale images). There are ten classes, namely, $G = \{0, 1, \ldots, 9\}$.



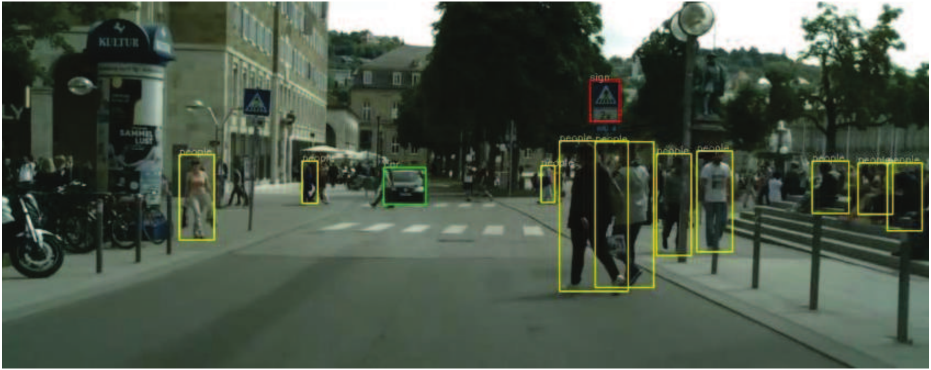
# Example: CIFAR-10 data set

The CIFAR-10 data set contains 60'000 image of size $32 \times 32$. There are ten classes, namely, $G = \{\texttt{airplane}, \texttt{automobile}, \ldots, \texttt{truck}\}$.



# Example: smart cars

Smart cars classify objects according to
$G \in \{$`cars, pedestrian, buildings, road signs, traffic lights,...`$\}$ and predict how these objects will move, and take decisions based on these predictions.




CES 2016: NVIDIA DRIVENet Demo - Visualizing a Self-Driving Future (part 5) (`www.youtube.com/watch?v=HJ58dbd5g8g`)

## What is the right model?

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*Everything should be made as simple as possible. But not simpler.*
[Albert Einstein; Physicist]

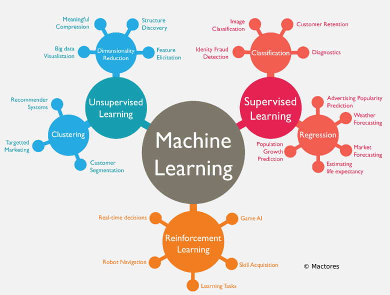
# In this course

(1) Statistical concepts

- Modeling, inference, prediction.
- Model assessment and selection: training versus test error, cross-validation, etc.

(2) Machine learning methods

- Regression: linear models, basis functions, regularization for high-dimensional data.
- Classification: linear methods, trees and random forest, support vector machines.
- Recent developments: convolutional (deep) neural networks, reinforcement learning, etc.



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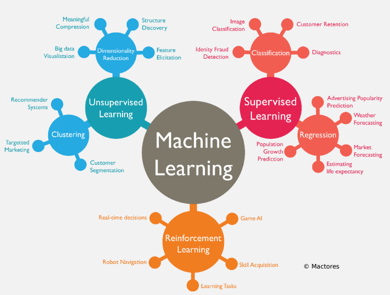


(3) Applications

- Analysis of simulated and real data sets.
- Image recognition

(4) Practical skills

- Programming with `python`.
- Working with data and interpretation of the results.