# Machine Learning Foundations

Inteligencia Artificial en los Sistemas de Control Autónomo
Máster Universitario en Ingeniería Industrial

Departamento de Automática

## Objectives

1. Define Machine Learning (ML)
2. Delimite ML scope
3. Introduce the main ML tasks
4. Recognize problems as ML tasks

## Bibliography


- Bishop, Christopher M. *Pattern Recognition and Machine Learning*. 2nd edition. Springer-Verlag. 2011
- Müller, Andreas C., Guido, Sarah. *Introduction to Machine Learning with Python*. 2nd edition. Springer-Verlag. 2011

# Table of Contents

# Introduction

## Justification

New opportunities

- Huge amount of new data sources: banking, social media, IoT, DNA, ...
- Increased computational power

New needs

- Manual data analysis is unfeasible
- Need of automatic methods

New goal

- Transform data into knowledge

# Introduction

## Definition (I)

### ML definition

ML is the science (and art) of programming computers so they can *learn from data*.

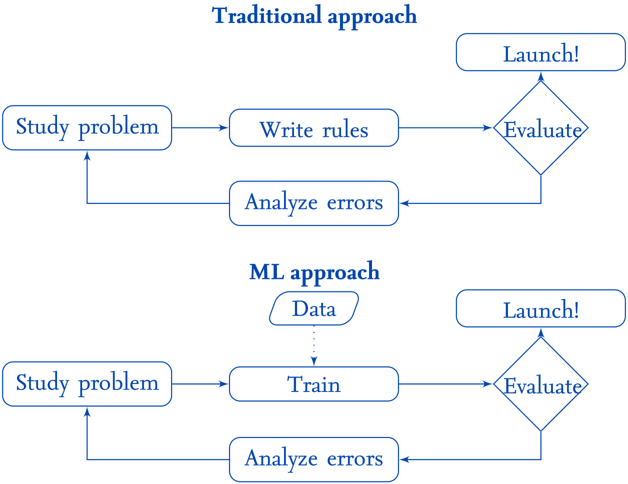
A. Géron, 2017

Alternative definitions

- Machine Learning is the field of study that gives computers the ability to learn without being explicitly programmed. Arthur Samuel, 1959.
- A computer program is said to learn from experience E with respect to some task T and some performance measure P, if its performance on T, as measured by P, improves with experience E. Tom Mitchell, 1997.

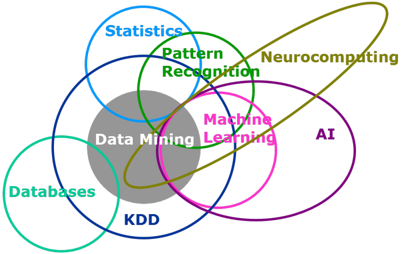
# Introduction

## Definition (II)



# Introduction

## The alphabet soup of data analysis



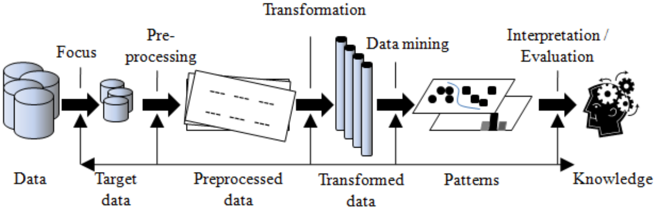

(Source)

Many related terms:

- Big Data
- Data Science
- Business Intelligence
- Data Mining
- Deep Learning
- Predictive analytics
- KDD
- Data scientist
- Data engineer
- ML engineer

# The data analysis process

## The big picture




(Source)

Steps in any ML application:

1. Data adquisition
2. Selection, cleaning and transformation
3. Machine Learning
4. Learning evaluation
5. Explotation

> The goal in ML is to get a representation of those patterns

# The data analysis process

## Data adquisition

Goal: Adquire data to perform ML

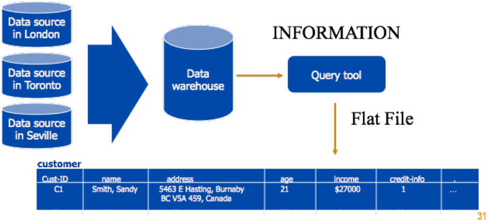
- From extremely easy -CSV file- to extremely complex -full Big Data system-

Public data repositories

- (Kaggle), (NASA Open Data Portal), (UCI Machine Learning Repository)

Customized adquisition and integration

- Integration from several data sources usually needed



# The data analysis process

## Selection, cleaning and transformation (I)

Goal: Prepare data for ML

- This phase is usually named preprocess

ML requires a clean data table

- Rows are named instances
- Columns are named features or attributes
- We refer the number of features as dimensionality

In some ML problems we use graphs instead of tables

| $f_1$ | $f_2$ | $\cdots$ | $f_n$ |
|---|---|---|---|
| $a_{1,1}$ | $a_{2,1}$ | $\cdots$ | $a_{n,1}$ |
| $a_{1,2}$ | $a_{2,2}$ | $\cdots$ | $a_{n,2}$ |
| $a_{1,3}$ | $a_{2,3}$ | $\cdots$ | $a_{n,3}$ |
| $a_{1,4}$ | $a_{2,4}$ | $\cdots$ | $a_{n,4}$ |
| $a_{1,5}$ | $a_{2,5}$ | $\cdots$ | $a_{n,5}$ |

# The data analysis process

## Selection, cleaning and transformation (II)

### Example: Bank data base

| IDC | Years | Euros | Salary | Own house | Defaults |
|---|---|---|---|---|---|
| 101 | 15 | 60000 | 2200 | Yes | 2 |
| 102 | 2 | 30000 | 3500 | Yes | 0 |
| 103 | 9 | 9000 | 1700 | Yes | 1 |
| 104 | 15 | 18000 | 1900 | No | 0 |
| ... | ... | ... | ... | ... | ... |

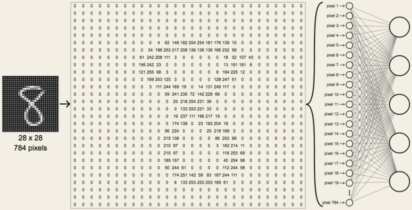
### Example: Robot sensors

| Timestamp | Sonar1 | Sonar2 | Sonar3 | Sonar4 |
|---|---|---|---|---|
| 1 | 1.687 | 0.445 | 2.332 | 0.429 |
| 2 | 0.812 | 0.481 | 1.702 | 0.473 |
| 3 | 1.572 | 0.471 | 1.654 | 0.513 |
| ... | ... | ... | ... | ... |

# The data analysis process

## Selection, cleaning and transformation (III)

### Example: Image recognition




(Source)

| Pixel1 | Pixel2 | Pixel3 | $\cdots$ | Pixel784 |
|---|---|---|---|---|
| 0 | 0 | 0 | $\cdots$ | 0 |
| $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ | $\cdots$ |
| 0 | 0 | 0 | $\cdots$ | 0 |

# The data analysis process

## Selection, cleaning and transformation (IV)

### Example: Text classification (bag-of-words representation)

1. Original text

```
(1) John likes to watch movies. Mary likes movies too.
(2) John also likes to watch football games.
```

2. Build list

```
(1) "John","likes","to","watch","movies","Mary","likes","movies","too"
(2) "John", also","likes","to","watch","football","games"
```

3. Build dictionary

```
(1) {"John":1,"likes":2,"to":1,"watch":1,"movies":2,"Mary":1,"too":1};
(2) {"John":1,"also":1,"likes":1,"to":1,"watch":1,"football":1,"games":1};
```

| John | likes | to | watch | movies | Mary | too | also | games | ⋯ |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2 | 1 | 1 | 2 | 1 | 1 | 0 | 0 | ⋯ |
| 1 | 1 | 1 | 1 | 0 | 0 | 0 | 1 | 1 | ⋯ |

# The data analysis process

## Selection, cleaning and transformation (V)

Preprocessing tasks

- Handle outliers (remove or leave them)
- Sample data (in case there are too much)
- Handle missing values
- Remove irrelevant or redundant features (for instance, social class and salary) feature selection
- Compute new attributes (get population density from area and population)
- Discretization, normalization, numerization, ...

# The data analysis process

## Machine Learning

Goal: Train an algorithm to perform a task

- As result, we obtain a model (or classifier or predictor depending on the context)

Machine Learning tasks

- Supervised learning: **classification** and regression
- Unsupervised learning: **clustering**, association, **dimensionality reduction** and anomality detection
- Reinforcement learning
- Many others

**No Free-Lunch Theorem**

No learning algorithm is a priori guaranteed to work better
More info: (D. Wolpert, 1996)

# The data analysis process

## Learning evaluation (I)

We do need to evaluate the trained model

- Models should perform well on new data

A naïve and wrong approach. Why is it wrong?

1. Train the model
2. Use the model to predict labels
3. Compute accuracy comparing predicted labels with known labels

Solution: Training and validation datasets

- **Training set**: Data used to train the models. Usually 70 %
- **Validation set**: Data used to validate the models. Usually 30 %
- Problems: Bias and loose of relevant data (serious in small datasets)

# The data analysis process

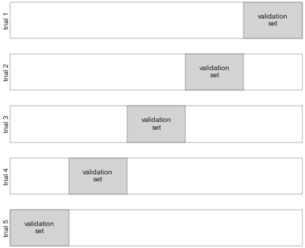
## Learning evaluation (II)

### Crossvalidation

1. Divide dataset in folds
2. Take one fold for validation
3. Train with the other folds
4. Validate and compute performance
5. Take another fold and repeat until finish
6. Average performance measures

Usually we use 10 folds

- 10-fold cross validation (or 10-CV)




(Source)

# The data analysis process

## Learning evaluation (III)

Select a measure to evaluate learning

- Proper measures depends on the problem

Classification learning measures

- Accuracy: Ratio of correct predictions
- F-Measure
- Confusion matrix
- ROC curve

Regression learning measures

- Mean Absolute Error (MAE)
- Mean Squared Error (MSE)
- $R^2$

Validation error must be taken, always, on the validation set

### Confusion matrix

| Actual class \ Predicted class | Class A | Class B | Class C |
|---|---|---|---|
| Class A | 100 | 0 | 10 |
| Class B | 10 | 80 | 10 |
| Class C | 30 | 0 | 70 |

(Source)

# The data analysis process

## Model exploitation

Model explotation depends on the objectives

- In Data Science, the model is interpreted and a report wroten
  - Formal report, bussiness intelligence dashboard, ...
- In Machine Learning, the model is integrated into a software system
  - Web application, app, robot controller, ...

The model may need maintenance

# Types of Machine Learning systems

## Overview

We can classify ML systems based on several (non-exclusive) criteria

- Whether or not they are trained with human supervision
  - Supervised, unsupervised, semisupervised and Reinforcement Learning
- Whether or not they can learn incrementally
  - Online vs. batch learning
- Whether they compare new data to known data
  - Instance-based vs. model-based learning
- The purpose of the system
  - Predictice models vs. explicative models
- The goal of the system
  - Discriminative models vs. generative models

We focus on supervised and unsupervised model-based discriminative batch algorithms.

# Types of Machine Learning systems
## Supervised learning (I)

In supervised learning input data comes along with the desired output

- Usually human beings label the output (named labels)

| $f_1$ | $f_2$ | $\cdots$ | $f_n$ | $y$ |
|---|---|---|---|---|
| $a_{1,1}$ | $a_{2,1}$ | $\cdots$ | $a_{n,1}$ | $y_1$ |
| $a_{1,2}$ | $a_{2,2}$ | $\cdots$ | $a_{n,2}$ | $y_2$ |
| $a_{1,3}$ | $a_{2,3}$ | $\cdots$ | $a_{n,3}$ | $y_3$ |
| $a_{1,4}$ | $a_{2,4}$ | $\cdots$ | $a_{n,4}$ | $y_4$ |
| $a_{1,5}$ | $a_{2,5}$ | $\cdots$ | $a_{n,5}$ | $y_5$ |

Two main tasks in supervised learning

- **Classification** if $y$ is a categorical attribute. Target attribute named class
- **Regression** if $y$ is numerical

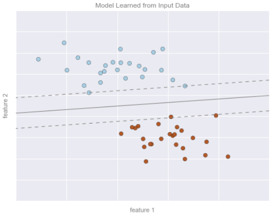
Advanced supervised learning tasks

- Semi-supervised learning, weakly supervised learning and multilabel classification

# Types of Machine Learning systems

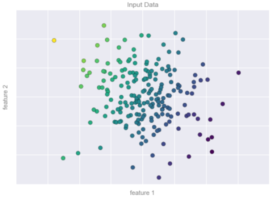
## Supervised learning (II)

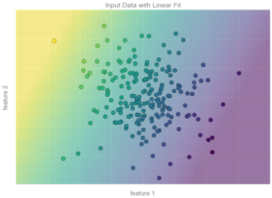
### Classification


(Source)

### Regression




(Source)

# Types of Machine Learning systems

## Supervised learning (III)

Important *classification* algorithms:

- k-Nearest Neighbors
- Support Vector Machines (SVMs)
- Decision Trees
    - ID3, C4.5 (J48), ...
- Rules
    - PART, CN2, AQ, ...
- Random Forests
- Bayesian Networks
- Neural Networks
- Ensambles

Important *regression* algorithms:

- Linear Regression
- Logistic Regression
- Symbolic Regression
- Regression trees
    - LM3 (M5), ...
- Neural Networks

# Types of Machine Learning systems

## Supervised learning: Classification (I)

Example: Bank credit risk management

| IDC | Years | Euros | Salary | Own house | Defaulter accounts | Returns credit |
|---|---|---|---|---|---|---|
| 101 | 15 | 60000 | 2200 | Yes | 2 | No |
| 102 | 2 | 30000 | 3500 | Yes | 0 | Yes |
| 103 | 9 | 9000 | 1700 | Yes | 1 | No |
| 104 | 15 | 18000 | 1900 | No | 0 | Yes |
| 105 | 10 | 24000 | 2100 | No | 0 | No |
| ... | ... | ... | ... | ... | ... | ... |

Objective: Predict if a customer would return a credit or not

# Types of Machine Learning Systems

## Supervised learning: Classification (II)

| Años | Euros | Salario | Casa propia | Cuentas morosas | Crédito |
|---|---|---|---|---|---|
| 10 | 50000 | 3000 | Si | 0 | ?? |

| Años | Euros | Salario | Casa propia | Cuentas morosas | Crédito |
|---|---|---|---|---|---|
| 15 | 60000 | 2200 | Si | 2 | No |
| 2 | 30000 | 3500 | Si | 0 | Si |
| 9 | 9000 | 1700 | Si | 1 | No |
| 15 | 18000 | 1900 | No | 0 | Si |
| 10 | 24000 | 2100 | No | 0 | No |
| | ... | ... | ... | ... | ... |

Algoritmo ML

**IF** CM >0 **THEN** NO

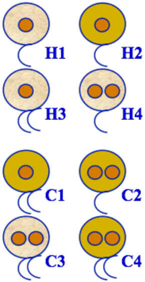
**IF** CM =0 **Y** S>2500 **THEN SI**

Crédito = Si

# Types of Machine Learning systems

## Supervised learning: Classification (III)

Example: Cancerous cells prediction

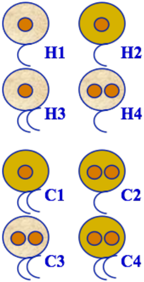



| ID | Colour | nuclei | tails | *class* |
|---|---|---|---|---|
| H1 | light | 1 | 1 | healthy |
| H2 | dark | 1 | 1 | healthy |
| H3 | light | 1 | 2 | healthy |
| H4 | light | 2 | 1 | healthy |
| C1 | dark | 1 | 2 | healthy |
| C2 | dark | 2 | 1 | healthy |
| C3 | light | 2 | 2 | healthy |
| C4 | dark | 2 | 2 | healthy |

# Types of Machine Learning systems

## Supervised learning: Classification (IV)

Example: Cancerous cells prediction



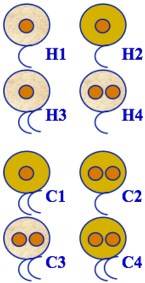

### Decision rules

```
^^I^^I^^Iif colour = light and nuclei =
    1
^^I^^I^^Ithen cell = healthy

^^I^^I^^Iif nuclei = 2 and colour = dark
^^I^^I^^Ithen cell = cancerours

^^I^^I^^I(and 4 rules more)
^^I    ^^I^^I
```

# Types of Machine Learning systems

## Supervised learning: Classification (V)

Example: Cancerous cells prediction



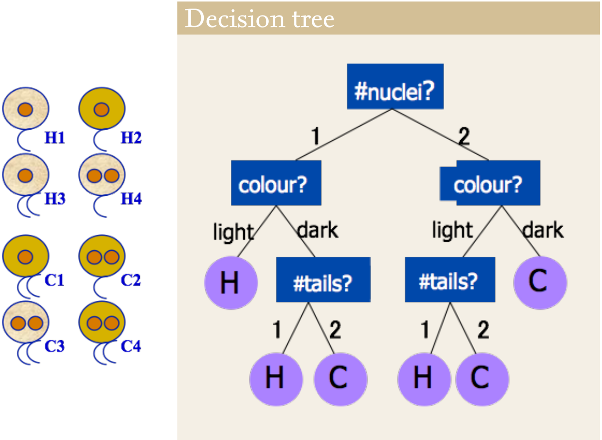

### Hierarchical decision rules

```
if colour = light and nuclei = 1
then cell = healthy

else
^^Iif nuclei = 2 and colour = dark
^^Ithen cell = cancerous

^^Ielse
^^I^^Iif tails = 1
^^I    then cell = healthy

^^I    else cell = cancerous
^^I   ^^I^^I
```

# Types of Machine Learning systems

## Supervised learning: Classification (VI)

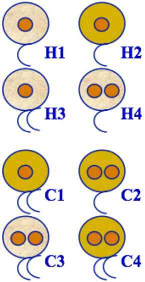
Example: Cancerous cells prediction



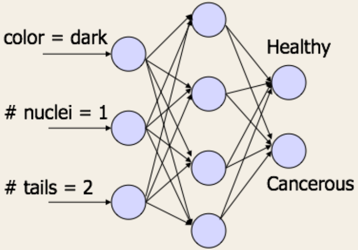
# Types of Machine Learning systems

## Supervised learning: Classification (VII)

Example: Cancerous cells prediction




### Neural network



# Types of Machine Learning systems

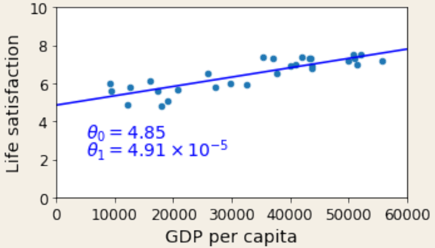
## Supervised learning: Regression (I)

Example: Does money make people happier? (example from (Géron, 2017))

| Country | GDP | *LS* |
|---|---|---|
| Hungary | 12,240 | 4.9 |
| Korea | 27,195 | 5.8 |
| France | 37,675 | 6.5 |
| Australia | 50,962 | 7.3 |
| USA | 55,805 | 7.2 |

LS =Life satisfaction

### Linear regression




$$\text{life\_satisfaction} = \theta_0 + \theta_1 \times \text{GDP\_per\_capita}$$

# Types of Machine Learning systems

## Unsupervised learning

In unsupervised learning there are no labels

| $f_1$ | $f_2$ | $f_3$ | $\cdots$ | $f_n$ |
|---|---|---|---|---|
| $a_{1,1}$ | $a_{2,1}$ | $a_{3,1}$ | $\cdots$ | $a_{n,1}$ |
| $a_{1,2}$ | $a_{2,2}$ | $a_{3,2}$ | $\cdots$ | $a_{n,2}$ |
| $a_{1,3}$ | $a_{2,3}$ | $a_{3,3}$ | $\cdots$ | $a_{n,3}$ |
| $a_{1,4}$ | $a_{2,4}$ | $a_{3,4}$ | $\cdots$ | $a_{n,4}$ |
| $a_{1,5}$ | $a_{2,5}$ | $a_{3,5}$ | $\cdots$ | $a_{n,5}$ |

Tasks in unsupervised learning

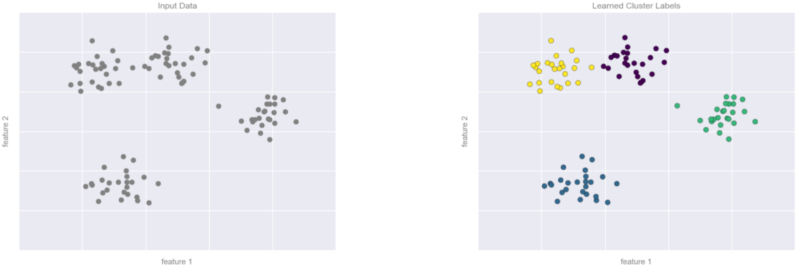
- Clustering
- Association rules
- Dimensionality reduction
- Anomality detection

# Types of Machine Learning systems

## Unsupervised learning: Clustering (I)

Clustering is a set of techniques that identify groups of data

- Algorithms: K-means, Expectation Maximization (EM), ...

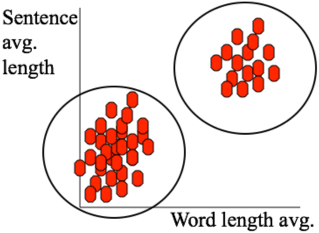



(Source)

# Types of Machine Learning systems

## Unsupervised learning: Clustering (II)

Example: Cluster word-sentence length in a books corpus




Clusters interpretation

- Long words and sentences: Philosophy?
- Short words and sentences: Novel?

# Types of Machine Learning systems

## Unsupervised learning: Clustering (III)

Example: Human resources department wants to know their employees profiles

| Salary | Married | Car | Child. | Rent/owner | Syndicated | Leaves | Sen. | Sex |
|---|---|---|---|---|---|---|---|---|
| 1000 | Yes | No | 0 | Rent | No | 7 | 15 | M |
| 2000 | No | Yes | 1 | Rent | Yes | 3 | 3 | F |
| 1500 | Yes | Yes | 2 | Owner | Yes | 5 | 10 | M |
| 3000 | Yes | Yes | 1 | Rent | No | 15 | 7 | F |
| 1000 | Yes | Yes | 0 | Owner | Yes | 1 | 6 | M |

# Types of Machine Learning systems

## Unsupervised learning: Clustering (IV)

| | Group 1 | Group 2 | Group 3 |
|---|---|---|---|
| Salary | 1535 | 1428 | 1233 |
| Married | 77 % | 98 % | 0 % |
| Car | 82 % | 1 % | 5 % |
| Child. | 0.05 | 0.3 | 2.3 |
| Rent/owner | 99 % | 75 % | 17 % |
| Syndicated | 80 % | 0 % | 67 % |
| Leaves | 8.3 | 2.3 | 5.1 |
| Seniority | 8.7 | 8 | 8.1 |
| Sex (M/F) | 61 % | 25 % | 83 % |

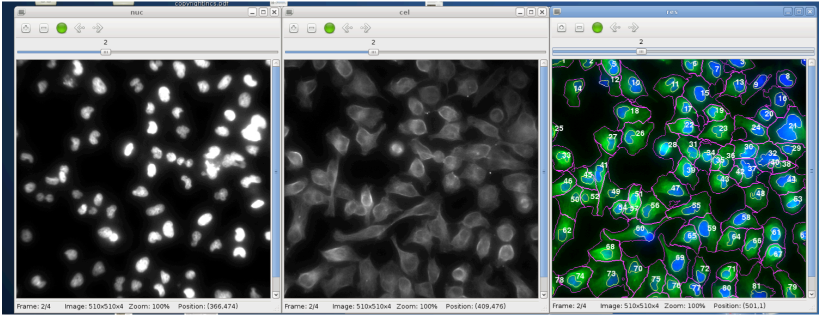
Analysis:

- Group 1: No children, with rented house. Low syndication. Many sick leaves.
- Group 2: No children, with car. High syndication. Low sick leaves. Usually women and rent.
- Group 3: With children, married, with car. Usually owners men. Low syndication.

# Types of Machine Learning systems

## Unsupervised learning: Clustering (V)

### Example: Cells number count



# Types of Machine Learning systems

## Unsupervised learning: Association rules (I)

Association rules seek relations among attributes

| $f_1$ | $f_2$ | $f_3$ | $\cdots$ | $f_n$ |
|---|---|---|---|---|
| $a_{1,1}$ | $a_{2,1}$ | $a_{3,1}$ | $\cdots$ | $a_{n,1}$ |
| $a_{1,2}$ | $a_{2,2}$ | $a_{3,2}$ | $\cdots$ | $a_{n,2}$ |
| $a_{1,3}$ | $a_{2,3}$ | $a_{3,3}$ | $\cdots$ | $a_{n,3}$ |
| $a_{1,4}$ | $a_{2,4}$ | $a_{3,4}$ | $\cdots$ | $a_{n,4}$ |
| $a_{1,5}$ | $a_{2,5}$ | $a_{3,5}$ | $\cdots$ | $a_{n,5}$ |

Main association algorithms

- Apriori, Eclat, GP-growth

Algorithm output

- Rules
- Confidence: How often the rule is true
- Support: How often the rule applies

# Types of Machine Learning systems

## Unsupervised learning: Association rules (II)

Example: Market basket analysis

- A supermarket wants to gather information about its clients shopping behaviour

Objective

- Identify complementary items
- Enhance product placement

| Id | Eggs | Oil | Diapers | Wine | Milk | Butter | Salmon | Lettuce | ... |
|---|---|---|---|---|---|---|---|---|---|
| 1 | Yes | No | No | Yes | No | Yes | Yes | Yes | ... |
| 2 | No | Yes | No | No | Yes | No | No | Yes | ... |
| 3 | No | No | Yes | No | Yes | No | No | No | ... |
| 4 | No | Yes | Yes | No | Yes | No | No | No | ... |
| 5 | Yes | Yes | No | No | No | Yes | No | Yes | ... |
| 6 | Yes | No | No | Yes | Yes | Yes | Yes | No | ... |
| 7 | No | No | No | No | No | No | No | No | ... |
| 8 | Yes | Yes | Yes | Yes | Yes | Yes | Yes | No | ... |
| ... | ... | ... | ... | ... | ... | ... | ... | ... | ... |

# Types of Machine Learning systems

## Unsupervised learning: Association rules (IV)

### Association rules

```
^^I^^I^^Iif diapers=si, then milk=yes
    (100%, 37%)
^^I^^I^^Iif eggs=yes, then oil=yes (50%,
    25%)
^^I^^I^^Iif wine=yes, then lettuce=yes
    (33%, 12%)
^^I    ^^I^^I
```

where (confidence, support)

# Types of Machine Learning systems

## Unsupervised learning: Dimensionality reduction (I)

Dimensionality reduction transforms data into more convenient representations

- Reduce data dimensionality
- Visualize multidimensional data

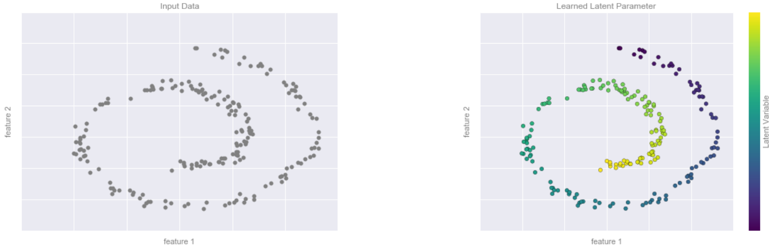
Main algorithms

- Isomap
- Principal Components Analysis (PCA)
- T-distributed Stochastic Neighbor Embedding (t-SNE)

# Types of Machine Learning systems

## Unsupervised learning: Dimensionality reduction (II)

### Example: Isomap

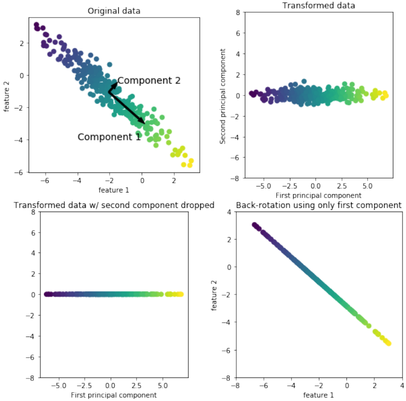



(Source)

# Types of Machine Learning systems

## Unsupervised learning: Dimensionality reduction (III)

### Example: PCA



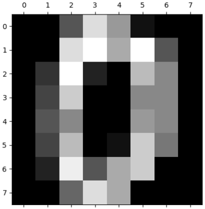

(Source)

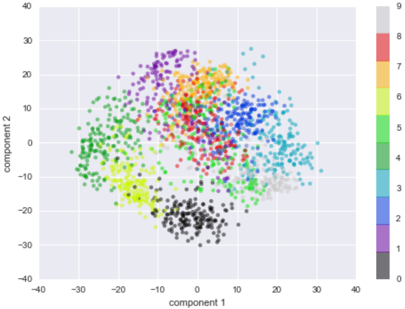
# Types of Machine Learning systems

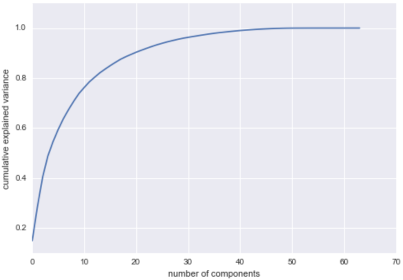
## Unsupervised learning: Dimensionality reduction (IV)

### Example: Hand-written digits recognition

- Images of hand-written digits
- 8x8 images (64 dimensions)
- 10 digits
- Classification problem



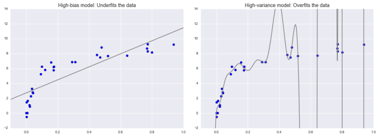



# Main challenges of Machine Learning

## Under and overfitting

Underfitting: Does not learn

- Topology too simple
- The model does not fit data
- Solution:
  - Increase model complexity




(Source)

Overfitting: Memorizes samples

- Topology too complex
- Very serious concern in ML
- The model does not generalize data
- Model fails when exposed to new data
- Solutions:
  - Reduce model complexity
  - Increase dataset
  - Apply regularization

# Main challenges of Machine Learning

## The curse of dimensionality

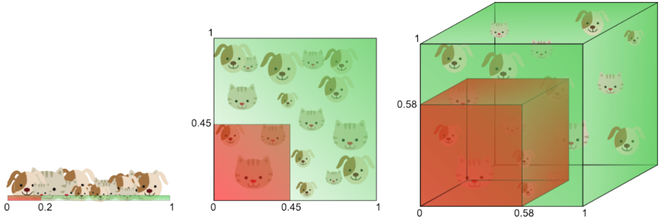
ML algorithms are statistical by nature

- Count frecuency of observations in regions

Fewer observations per region as dimensionality increases

- Data become sparser
- Need of more data to keep patterns
- Increased overfitting risk

Goal: Reduce dimensionality as much as possible

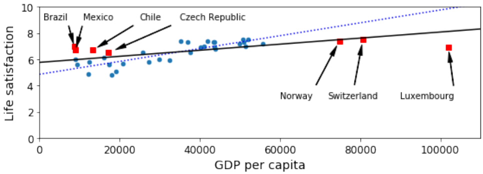



(Source)

# Main challenges of Machine Learning

## Other challenges

- Insufficient data
  - Given enough data, algorithms tend to similar performance
  - Remember: ML is data-centric
- Non representative training data
- Poor quality data
- Irrelevant features
- Unbalanced datasets




(Source)

# Case studies

## Case study 1: Bank propensity model

Client

- Bank

Business problem

- Identify those clients prone to buy a service

Data

- Available on several databases
- Historical data on service adquisition available

Propose a solution to:

- Data adquisition
- ML task
- Predictive or explicative model
- Model explotation
- Model maintenance

# Case studies

## Case study 2: Social media compaign impact

Client

- Car manufacturer

Business problem

- Real-time analysis of a campaign impact in Twitter
- Answer if people have a positive reaction to the campaign

Data

- None

Propose a solution to:

- Data adquisition
- ML task
- Predictive or explicative model
- Model explotation
- Model maintenance

# Case studies

## Case study 3: Hubble FGS-3 servo failure prediction

Client

- NASA

Business problem

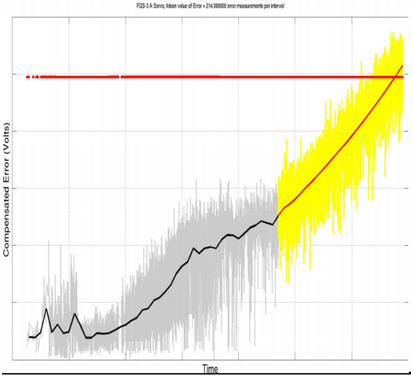
- Predict Hubble FGS-3 servo failure

Data

- Compensated error telemetry
- Servo will fail if compensated error exceeds a threshold

Propose a solution to:

- ML task
- Predictive or explicative model
- Model explotation
- Model maintenance




(Source of this study case)

# Case studies

## Case study 4: Fall detection with triaxial accelerometer

Client

- Technological start-up

Business problem

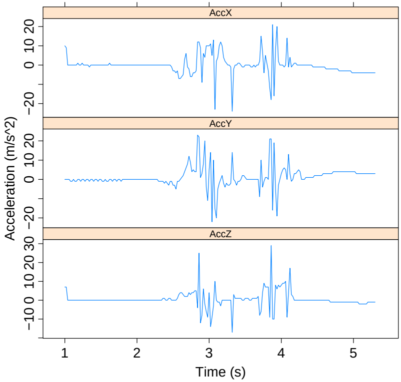
- Detect falls with a smartwatch
- Improve elderly people attention

Data

- None

Propose a solution to:

- Data adquisition
- ML task
- Data preprocessing
- Model explotation
- Model maintenance




(More info)

# Case studies

## Case study 5: Fall detection with sound

Client

- Technological start-up

Business problem

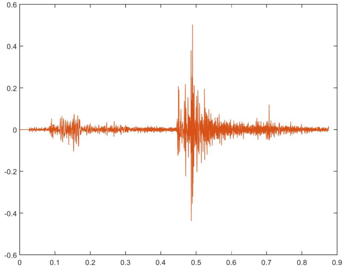
- Detect falls with sound
- Improve elderly people attention

Data

- None

Propose a solution to:

- Data adquisition
- ML task
- Data preprocessing
- Model explotation
- Model maintenance




| | |
|---|---|
| Energy Mean | Energy Std |
| Number of Zeros Mean | Number of Zeros Std |
| Spectral Flux Mean | Spectral Flux Std |
| Roll off Factor Mean | Roll off Factor Std |
| Spectral centroid Mean | Spectral Centroid Std |

(More info)