Machine Learning Foundations

Inteligencia Artificial en los Sistemas de Control Autónomo
Máster en Ciencia y Tecnología desde el Espacio

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

- Géron, Aurélien. *Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow*. 2nd edition. O'Reilly. 2019
- Müller, Andreas C., Guido, Sarah. *Introduction to Machine Learning with Python*. O'Reilly. 2016

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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*.

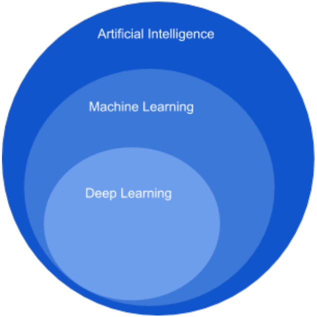
A. Géron, 2017

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

The alphabet soup of data analysis



(Source)

Many related terms

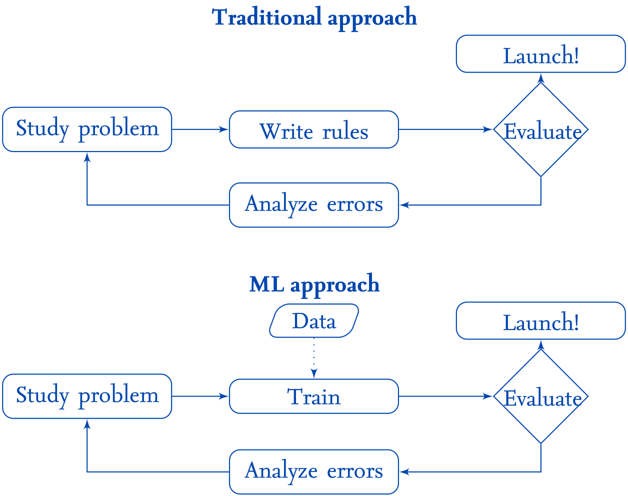
- Artificial Intelligence
- Machine Learning
- Deep Learning
- Big Data

And new careers

- Data Science
- Data scientist
- Data engineer
- ML engineer

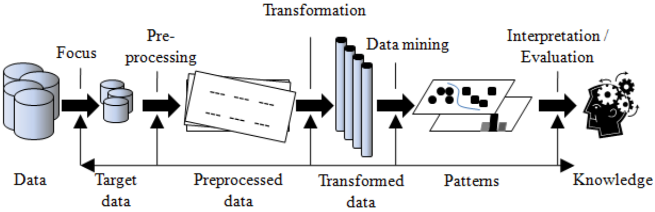
Introduction

Definition (II)



The data analysis process

The big picture



(Source)

Steps in any ML application:

1. Data adquisition
2. Selection, cleaning and transformation (preprocessing)
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

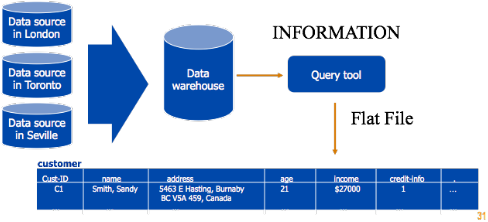
- From extremely easy -CSV file- to extremely complex -full Big Data system-

Public data repositories

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

Customized adquisition and integration

- Integration from several data sources usually needed



The data analysis process

Data adquisition: Space data sources

Data sources highly dependent on domain and mission

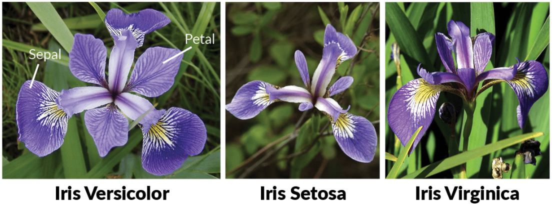
- Many missions have their own website to download data
- Each mission contains data from different instruments

There are, however, some integrated data products sources

- (OMNIWeb) - Heliophysics / Space Weather
- (CDAWeb) - Non-solar Heliophysics
- (SSCWeb) - Satellite situation
- (Heliophysics Data Portal) - Heliophysics
- (HAPI) - “Integration of integrated” data sources
- Python packages
  - SunPy, AstroPy, SpacePy, PySat, PySPEDAS, etc

The data analysis process

Data adquisition: Famous datasets - Iris (I)



Iris dataset

- First used by Roland Fisher in 1936
- Classification problem: three iris species
- Balanced dataset: 150 instances, three classes, 50 instances each
- Four attributes (petal width, petal length, sepal width, sepal length)

The data analysis process

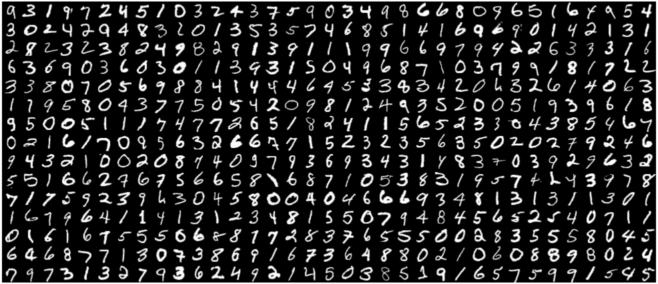
Data adquisition: Famous datasets - Iris (II)

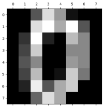
	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa
...	...	...	...	...	...
145	6.7	3.0	5.2	2.3	Iris-virginica
146	6.3	2.5	5.0	1.9	Iris-virginica
147	6.5	3.0	5.2	2.0	Iris-virginica
148	6.2	3.4	5.4	2.3	Iris-virginica
149	5.9	3.0	5.1	1.8	Iris-virginica

(More info in Kaggle)

The data analysis process

Data adquisition: Famous datasets - MNIST





Hand-written digit recognition

- 60,000 training samples, 10,000 test samples
- 8x8 images
- 10 classes
- (More in Kaggle)

The data analysis process

Data adquisition: data file formats - CSV

CSV (Comma-Separated Values)

- Text format for tabular data
- Editable with system tools and Excel
- Rows store records
- Columns store attributes
- Fields are separated by commas

Year	Make	Model	Description	Price
1997	Ford	E350	ac, abs, moon	3000.00
1999	Chevy	Venture "Extended Edition"		4900.00
1999	Chevy	Venture "Extended Edition, Very Large"		5000.00
1996	Jeep	Grand Cherokee	MUST SELL! air, moon roof, loaded	4799.00

filename.csv

```
Year,Make,Model,Description,Price
1997,Ford,E350,"ac, abs, moon",3000.00
1999,Chevy,"Venture ""Extended Edition""","",4900.00
1999,Chevy,"Venture ""Extended Edition, Very Large""","",5000.00
1996,Jeep,Grand Cherokee,"MUST SELL!
air, moon roof, loaded",4799.00
```

The data analysis process

Data adquisition: data file formats - JSON

JSON: Data format for hierarchical data

- Created in 2001 for stateless client-server communication
- Text-based
- Complex data structures

filename.json

```json
{
  "firstName": "John",
  "isAlive": true,
  "age": 27,
  "address": {
    "streetAddress": "21 2nd Street",
    "city": "New York",
    "state": "NY",
  },
  "phoneNumbers": [
    {
      "type": "home",
      "number": "212 555-1234"
    },
    {
      "type": "office",
      "number": "646 555-4567"
    }
  ]
}
```

The data analysis process

Data adquisition: data file formats - Space data

Several formats designed for space applications

- NASA CDF (*Common Data Format*)
  - (More info)
- FITS (*Flexible Image Transport System*)
  - Astronomical image format supported by NASA and IAU
  - (More info)
- HDF5: Big Data format, not specific for space

Specific tools for files manipulation and loading

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
...	...	...	...	...	...

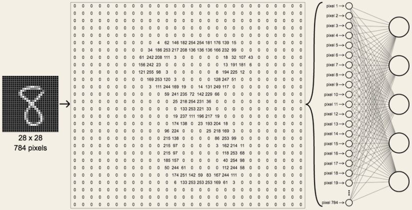
Example: Robot sensors

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	...	Pixel784
o	o	o	...	o
...	...	...	...	...
o	o	o	...	o

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 (feature selection)
  - For instance, attributes "social class" and "salary" contain highly correlated information
- Compute new attributes (feature engineering)
  - For instance, compute "population density" from "area" and "population"
- Transform attributes
  - Discretization, normalization, numerization, ...

The data analysis process

Data processing levels

Three levels of processing for data products in space applications

- Level 0: Unprocessed data from payload
- Level 1: Processed data
- Level 2: Processed data with geophysical variables

(More info)

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 training methods (or ML 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

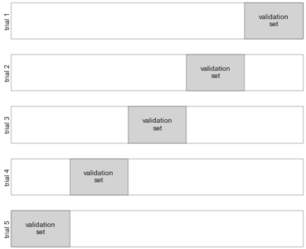
Learning evaluation (II)

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)



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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 supervision
  - Supervised, unsupervised, semisupervised and Reinforcement Learning
- Whether or not they can learn incrementally
  - Online vs. batch learning
- When forecasting is done
  - Nowcasting vr. forecasting
- Type of analytics
  - Descriptive, predictive or prescriptive
- The goal of the system
  - Discriminative models vs. generative models
- The interpretation of the model
  - Predictive models (blackbox) vs. explicative models (whitebox)

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

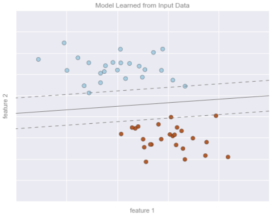
Advanced supervised learning tasks

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

Types of Machine Learning systems

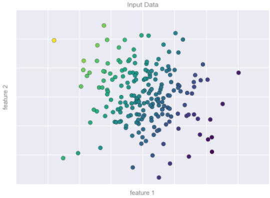
Supervised learning (II)

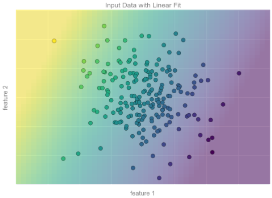
Classification



(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

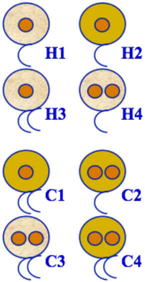
IF CM =0 **Y** S>2500 **THEN** SI

Crédito = Si

Types of Machine Learning systems

Supervised learning: Classification (III)

Example: Cancerous cells prediction

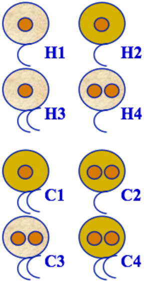


ID	Colour	nuclei	tails	*class*
H1	light	1	1	*healthy*
H2	dark	1	1	*healthy*
H3	light	1	2	*healthy*
H4	light	2	1	*healthy*
C1	dark	1	2	*cancer*
C2	dark	2	1	*cancer*
C3	light	2	2	*cancer*
C4	dark	2	2	*cancer*

Types of Machine Learning systems

Supervised learning: Classification (IV)

Example: Cancerous cells prediction



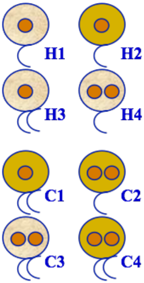
Decision rules

```
if colour = light and nuclei = 1
then cell = healthy ^^I
^^I^^I^^I
if nuclei = 2 and colour = dark
then cell = cancerours

(and 4 rules more)
```

Types of Machine Learning systems

Supervised learning: Classification (V)

Example: Cancerous cells prediction



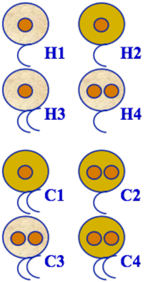
Hierarchical decision rules

```
if colour = light and nuclei = 1
then cell = healthy   ^^I
^^I^^I^^I
else
    if nuclei = 2 and colour = dark
    then cell = cancerous

   else
       if tails = 1
       then cell = healthy

       else cell = cancerous
```

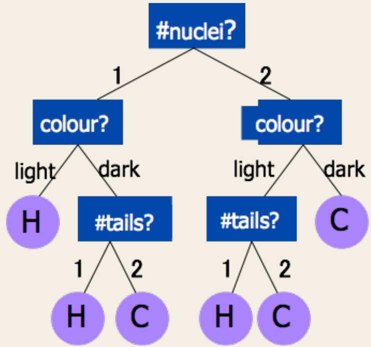
Types of Machine Learning systems

Supervised learning: Classification (VI)

Example: Cancerous cells prediction



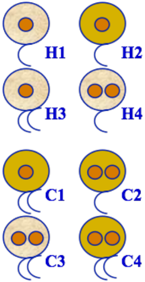
Decision tree

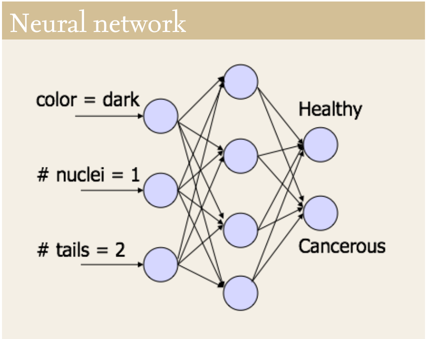


Types of Machine Learning systems

Supervised learning: Classification (VII)

Example: Cancerous cells prediction





Types of Machine Learning systems

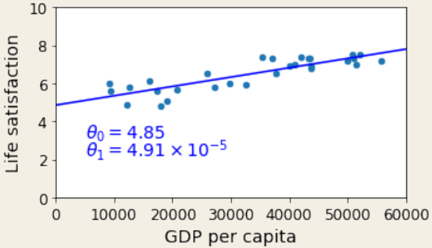
Supervised learning: Regression (I)

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

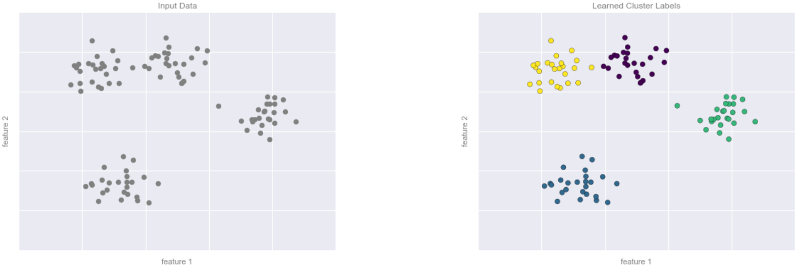
- Clustering
- Association rules
- Dimensionality reduction
- Anomality detection

Types of Machine Learning systems

Unsupervised learning: Clustering (I)

Clustering is a set of techniques that identify groups of data (clusters)

- Algorithms: K-means, db-scan, Gaussian Mixture Models (GMM), Expectation Maximization (EM), ...

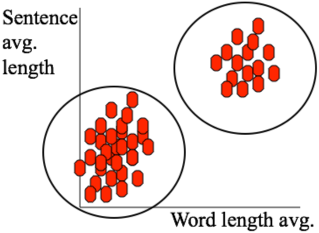


(Source)

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 %

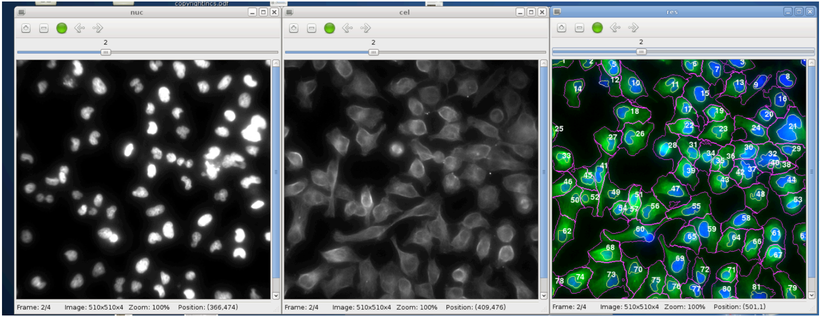
Analysis:

- 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

```
if diapers=yes
then milk=yes (100%, 37%)

if eggs=yes
then oil=yes (50%, 25%)

if wine=yes
then lettuce=yes (33%, 12%)
```

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

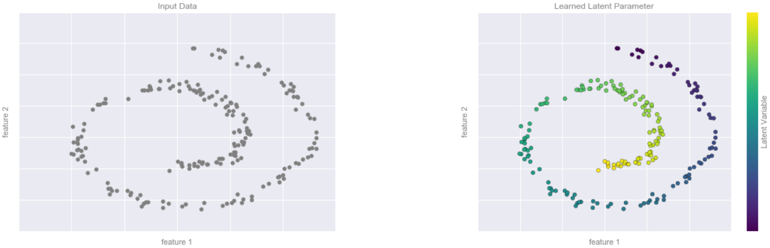
Main algorithms

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

Types of Machine Learning systems

Unsupervised learning: Dimensionality reduction (II)

Example: Isomap



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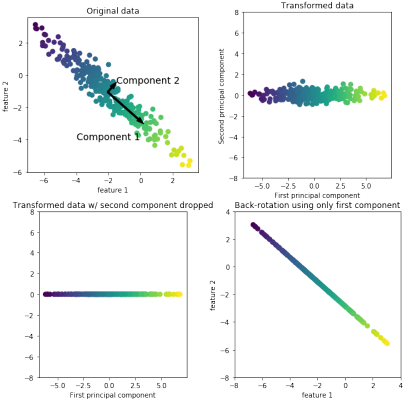
Types of Machine Learning systems

Unsupervised learning: Dimensionality reduction (III)

Example: PCA



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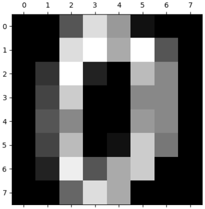
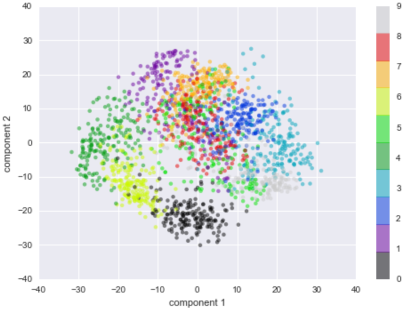
Types of Machine Learning systems

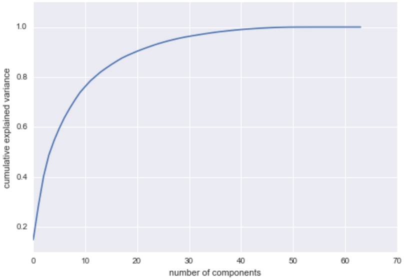
Unsupervised learning: Dimensionality reduction (IV)

Example: Hand-written digits recognition

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





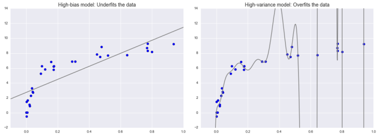


Main challenges of Machine Learning

Under and overfitting

Underfitting: Does not learn

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



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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

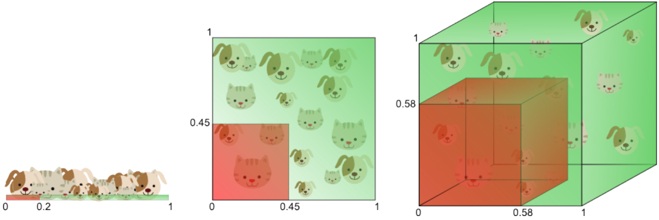
ML algorithms are statistical by nature

- 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



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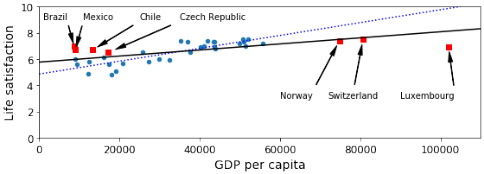
Main challenges of Machine Learning

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



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