Machine Learning Foundations

Aprendizaje Automático para la Robótica Máster Universitario en Ingeniería Industrial

Departamento de Automática





Objectives

- 1. Define Machine Learning (ML)
- 2. Delimite ML scope
- 3. Introduce the main ML tasks4. 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. O'Reilly. 2016

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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

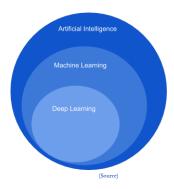
Alternative definitions

- 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



Many related terms

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

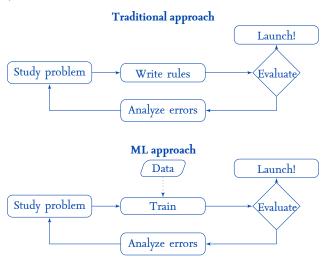
And new careers

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



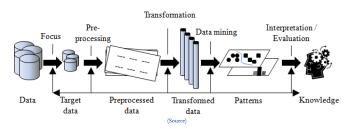
Introduction

Definition (II)





The big picture



Steps in any ML application:

- 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

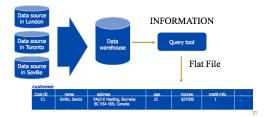
• From extremely easy -CSV file- to extremely complex -full Big Data system-

Public data repositories

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

Customized adquisition and integration

Integration from several data sources usually needed





The data analysis process

Data adquisition: Famous datasets - Iris (I)







Iris Versicolor

Iris Setosa

Iris Virginica

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)

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)



Data adquisition: Famous datasets - MNIST





Hand-written digit recognition

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



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
```



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

```
"firstName": "John",
"is Alive": 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

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		f_n
$\mathfrak{a}_{1,1}$	$\mathfrak{a}_{2,1}$	• • •	$\mathfrak{a}_{\mathfrak{n},1}$
$\mathfrak{a}_{1,2}$	$\mathfrak{a}_{2,2}$	• • •	$\mathfrak{a}_{\mathfrak{n},2}$
$\mathfrak{a}_{1,3}$	$\mathfrak{a}_{2,3}$	• • •	$\mathfrak{a}_{\mathfrak{n},3}$
$\mathfrak{a}_{1,4}$	$\mathfrak{a}_{2,4}$	• • •	$\mathfrak{a}_{\mathfrak{n},4}$
$\mathfrak{a}_{1,5}$	$\mathfrak{a}_{2,5}$	• • •	$a_{n,5}$



Selection, cleaning and transformation (II)

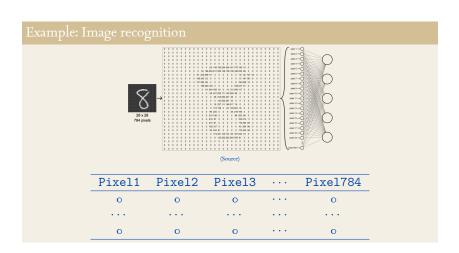
IDC	Years	Euros	Salary	Own house	Defaults
IOI	15	60000	2200	Yes	2
102	2	30000	3500	Yes	O
103	9	9000	1700	Yes	I
104	15	18000	1900	No	O

Timestamp	Sonar1	Sonar2	Sonar3	Sonar4
I	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)





Selection, cleaning and transformation (IV)

Original text

- (I) John likes to watch movies. Mary likes movies too.
- (2) John also likes to watch football games.

2. Build list

- (I) "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	• • •
I	2	I	I	2	I	I	О	О	
I	I	I	I	O	O	O	I	I	



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

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)



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?

- T. 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)



Learning evaluation (II)

Crossvalidation

- T. 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)



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)
- R²

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

C	onf	usion m	atrix			
			Pred	icted cl	ass	
			Class A	Class B	Class C	
	ars.	Class A	100	О	IO	
	Actual class	Class B	10	8o	10	
(So:		Class C	30	О	70	



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



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)



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	• • •	fn	Υ
$\mathfrak{a}_{1,1}$	$\mathfrak{a}_{2,1}$	• • •	$\mathfrak{a}_{\mathfrak{n},1}$	γ1
$\mathfrak{a}_{1,2}$	$\mathfrak{a}_{2,2}$	• • •	$\mathfrak{a}_{\mathfrak{n},2}$	γ2
$\mathfrak{a}_{1,3}$	$\mathfrak{a}_{2,3}$	• • •	$\mathfrak{a}_{\mathfrak{n},3}$	ү з
$\mathfrak{a}_{1,4}$	$\mathfrak{a}_{2,4}$	• • •	$\mathfrak{a}_{\mathfrak{n},4}$	γ4
$\mathfrak{a}_{1,5}$	$\mathfrak{a}_{2,5}$	• • •	$a_{n,5}$	γ5

Two main tasks in supervised learning

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

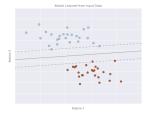
Advanced supervised learning tasks

 Semi-supervised learning, weakly supervised learning and multilabel classification



Supervised learning (II) Classification

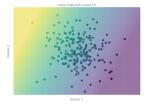




(Source)

Regression





(Source)



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
- Epsambles

Important regression algorithms:

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



Supervised learning: Classification (I)

Example: Bank credit risk management

IDC	Years	Euros	Salary	Own house	Defaulter accounts	Returns credit
IOI	15	60000	2200	Yes	2	No
102	2	30000	3500	Yes	O	Yes
103	9	9000	1700	Yes	I	No
104	15	18000	1900	No	O	Yes
105	IO	24000	2100	No	O	No

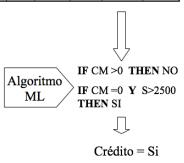
Objective: Predict if a customer would return a credit or not



Supervised learning: Classification (II)

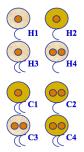
Años	Euros	Salario		Cuentas morosas	Crédito
10	50000	3000	Si	0	??

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



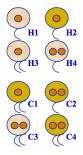


Supervised learning: Classification (III)



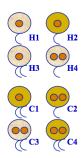
ID	Colour	nuclei	tails	class
Н1	light	I	I	healthy
H_2	dark	I	I	healthy
H_3	light	I	2	healthy
H_4	light	2	I	healthy
$C_{\mathbf{I}}$	dark	I	2	cancer
C_2	dark	2	I	cancer
C_3	light	2	2	cancer
C ₄	dark	2	2	cancer

Supervised learning: Classification (IV)



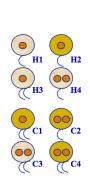
```
if colour = light and nuclei = 1
then cell = healthy ^^I
\vee \vee \perp \vee \vee \perp \vee \vee \perp
if nuclei = 2 and colour = dark
then cell = cancerours
(and 4 rules more)
```

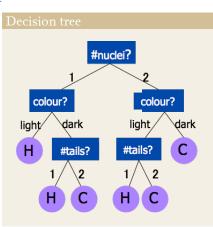
Supervised learning: Classification (V)



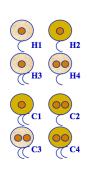
```
if colour = light and nuclei = 1
then cell = healthy
\vee \vee \vee \vee \vee \vee \vee \vee \vee
else
     if nuclei = 2 and colour = dark
     then cell = cancerous
   else
          if tails = T
          then cell = healthy
          else cell = cancerous
```

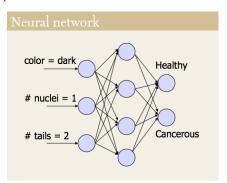
Supervised learning: Classification (VI)





Supervised learning: Classification (VII)



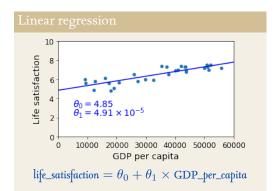


Supervised learning: Regression (I)

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





Unsupervised learning

In unsupervised learning there are no labels

f ₁	f_2	f3	• • •	fn
$\mathfrak{a}_{1,1}$	$\mathfrak{a}_{2,1}$	$\mathfrak{a}_{3,1}$	• • •	$\mathfrak{a}_{\mathfrak{n},1}$
$\mathfrak{a}_{1,2}$	$\mathfrak{a}_{2,2}$	$\mathfrak{a}_{3,2}$	• • •	$\mathfrak{a}_{\mathfrak{n},2}$
$\mathfrak{a}_{1,3}$	$\mathfrak{a}_{2,3}$	$\mathfrak{a}_{3,3}$	• • •	$\mathfrak{a}_{\mathfrak{n},3}$
$\mathfrak{a}_{1,4}$	$\mathfrak{a}_{2,4}$	$\mathfrak{a}_{3,4}$	• • •	$\mathfrak{a}_{\mathfrak{n},4}$
$\mathfrak{a}_{1,5}$	$\mathfrak{a}_{2,5}$	$\mathfrak{a}_{3,5}$	• • •	$a_{n,5}$

Tasks in unsupervised learning

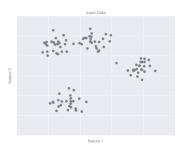
- Clustering
- Association rules
- Dimensionality reduction
- Anomality detection

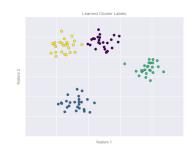


Unsupervised learning: Clustering (I)

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

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



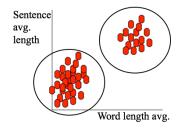


(Source)



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?



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	O	Rent	No	7	15	M
2000	No	Yes	I	Rent	Yes	3	3	F
1500	Yes	Yes	2	Owner	Yes	5	IO	M
3000	Yes	Yes	I	Rent	No	15	7	F
1000	Yes	Yes	O	Owner	Yes	I	6	M

Unsupervised learning: Clustering (IV)

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

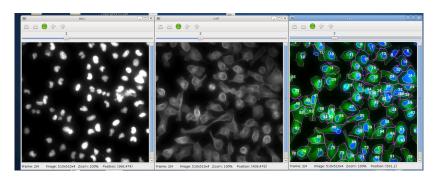
Analysis:

- 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.



Unsupervised learning: Clustering (V)

Example: Cells number count





Unsupervised learning: Association rules (I)

Association rules seek relations among attributes

f_1	f_2	f3		f_n
$\mathfrak{a}_{1,1}$	$\mathfrak{a}_{2,1}$	$\mathfrak{a}_{3,1}$		$\mathfrak{a}_{\mathfrak{n},1}$
$\mathfrak{a}_{1,2}$	$\mathfrak{a}_{2,2}$	$\mathfrak{a}_{3,2}$	• • •	$\mathfrak{a}_{\mathfrak{n},2}$
$\mathfrak{a}_{1,3}$	$\mathfrak{a}_{2,3}$	$\mathfrak{a}_{3,3}$	• • •	$\mathfrak{a}_{\mathfrak{n},3}$
$\mathfrak{a}_{1,4}$	$\mathfrak{a}_{2,4}$	$\mathfrak{a}_{3,4}$	• • •	$\mathfrak{a}_{\mathfrak{n},4}$
$\mathfrak{a}_{1,5}$	$\mathfrak{a}_{2,5}$	$\mathfrak{a}_{3,5}$	• • •	$a_{n,5}$

Main association algorithms

Apriori, Eclat, GP-growth

Algorithm output

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



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	
I	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	



```
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)

Unsupervised learning: Dimensionality reduction (I)

Dimensionality reduction transforms data into more convenient representations

- Reduce data dimensionality
- Visualize multidimensional data

Main algorithms

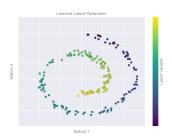
- Isomap
- Principal Components Analysis (PCA)
- T-distributed Stochastic Neighbor Embedding (t-SNE)



Unsupervised learning: Dimensionality reduction (II)

Example: Isomap

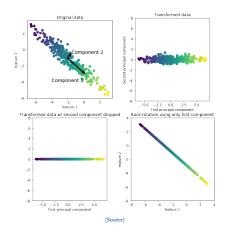




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Unsupervised learning: Dimensionality reduction (III)

Example: PCA

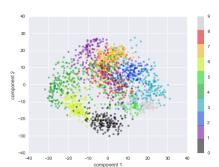


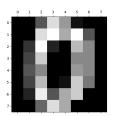


Unsupervised learning: Dimensionality reduction (IV)

Example: Hand-written digits recognition

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







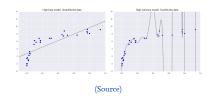


Main challenges of Machine Learning

Under and overfitting

Underfitting: Does not learn

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



Overfitting: Memorizes samples

- Topology too complex
- Very serious concern in ML
- The model does not generalize data
- Model fails when exposed to new data

Main challenges of Machine Learning

- Solutions:
 - Reduce model complexity
 - Increase dataset
 - Apply regularization



Main challenges of Machine Learning

The curse of dimensionality

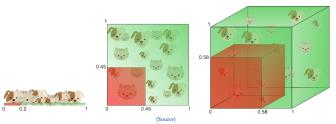
ML algorithms are statistical by nature

• 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

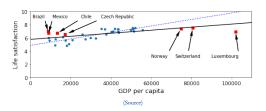




Main challenges of Machine Learning

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





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

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



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

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



Case study 3: Hubble FGS-3 servo failure prediction

Client

NASA

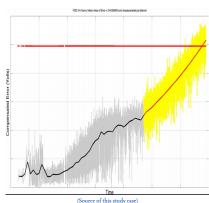
Business problem

• Predict Hubble FGS-3 servo failure

Data

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

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





Case study 4: Fall detection with triaxial accelerometer

Client

• Technological start-up

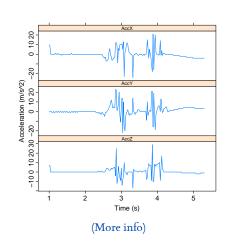
Business problem

- Detect falls with a smartwatch
- Improve elderly people attention

Data

None

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





Case study 5: Fall detection with sound

Client

Technological start-up

Business problem

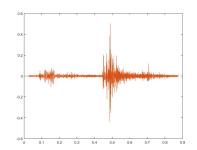
- Detect falls with sound
- Improve elderly people attention

Data

None

Propose a solution to:

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



Energy Mean Number of Zeros Mean Spectral Flux Mean Roll off Factor Mean Spectral centroid Mean

Energy Std Number of Zeros Std Spectral Flux Std Roll off Factor Std Spectral Centroid Std

(More info)



Case study 6: NASA JPL BioSleeve

Client

NASA JPL Advanced Robotics Group

Business problem

• Recognize hand gestures (more info)

Data

None

Propose a solution to:

- Data adquisition
- ML task



(Source)



(Source)

Wolf, Michael T., et al. Decoding static and dynamic arm and hand gestures from the JPL BioSleeve. IEEE Aerospace Conference. IEEE, 2013.

(Solution) (Results)



Case study 7: UAV terrain classification

Client

• NASA JPL Advanced Robotics Group

Business problem

- Recognize terrain type for automatic UAV landing
- (Video)

Data

- UAV down-looking camera
- No dataset available

- Data adquisition
- ML task
- Feature extraction

