Bruno Agard

WORKSHOP #3
MACHINE LEARNING FOR PREDICTIVE ANALYSIS

PARTNER IN GROWTH HEC MONTRÉAL

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WELCOME

Workshop#3
Machine Learning for Predictive Analysis

Session#	Day	Date
11	Tuesday	sept. 15th
12	Wednesday	sept. 16th
13	Thursday	sept. 17th
14	Tuesday	sept. 22nd

Start: 1:30 pm

End: 4:30

ERICSSON

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YOUR INSTRUCTOR

Bruno Agard
DEA, Ph.D
Professor Polytechnique Montréal,
Department of Mathematics and industrial engineering

EXPERTISE

- Industrial engineering
- Information technology
- Artificial Intelligence
- Industry 4.0

OTHER PROFESSIONAL IMPLICATIONS:

- Director, laboratory in data intelligence
- Member, laboratory Poly-Industries 4.0
- Member, interuniversity Research Centre CIRRELT
- Member, Canada Research Chair on personal mobility Member , Institute for Data Valorization (IVADO)
- Member, Centre interdisciplinaire de recherche en opérationnalisation du développement durable (CIRODD)

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Workshop#3
Machine Learning for Predictive Analysis

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11	Tuesday	sept. 15th	Start: 1:30 pm
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- Essentials of linear and logistic regression models
- Methods for evaluating the performance of predictive models (learning-validation-test data; cross-validation; ROC curve)
- Regression and classification tree
- Random forest
- « Gradient boosting »
- Neural network – Introduction to multilayer perceptron neural networks

Workshop#4
Non supervised Machine Learning

Session#	Day	Date	
15	Wednesday	sept.23rd	Start: 1:30 pm
16	Thursday	sept. 25th	End: 4:30
17	Tuesday	sept. 29th	
18	Wednesday	sept. 30th	

- Grouping / segmentation analysis: hierarchical and non-hierarchical methods, mixed methods
- Introduction to association rules, methods based on nearest neighbors, filtering methods
- Applications of non-supervised methods to anomaly detection
- Data preparation

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ONLINE TRAINING TIPS

HEC MONTRÉAL

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MAKE THE MOST OF YOUR EXPERIENCE

Keep your microphone on mute when you are not participating

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PARTICIPATE THROUGHOUT THE TRAINING

Use the **Raise Hand** feature to ask a question

Interact in the **Chat** window

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MATERIAL YOU SHOULD HAVE

- One pdf file with actual presentation
  - HEC #3.pdf
- One Python Jupyter Notebook file
  - HEC #3.ipynb
- Some data files
  - Reg_1.csv, Class_1.csv
- One computer with
  - Python Jupyter installed
  - The following libraries installed : pandas, numpy, sklearn

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HOW TO START

1. Start a Python Jupyter Notebook session
2. Load the Python file provided for the Workshop
   - HEC #3.ipynb
3. Identify the path where the data files are located
   - Reg_1.csv, Class_1.csv
4. Update the path variable to find your data file
   - path='../usermane/Desktop/Data/'
5. Run the first block of code, if the head of the file "Reg_1.csv » appers, your in ☺

Step -1

Before to start

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INTRODUCTION

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TABLE

- Lines : object / item / customers
- Columns : attributes / variables
- Data :
  - Type : discrete / continuous
  - Value : N/A, U, missing,

Customer	Sexe	Age	Adress	City	Paiement mode	Active
#1	M	35	« 34 St. Denis »	Montréal	Interact	yes
#2	F	27	« 15 bis. Main St. »	Toronto	Credit Card	yes
…	…	…	…	…	…	…
#654332	U	56	« 250 Av. Champlain »	Québec	Interact	no

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DATABASE

- Set of tables

Customer table

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#1	M	35	« 34 St. Denis »	Montréal	Interact	yes
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…	…	…	…	…	…	…
#654332	U	56	« 250 Av. Champlain »	Québec	Interact	no

Product ref table

Cust.	Intern ref.	Name	Date
#1	#P1564	Phone model 1	date 1
#1	#P3684	Phone model 5	date 3
#1	#MG3685	Modem G	date 3
#1	#VF543699	Video recorder F	date 3
#2	#P985	Phone model 3	date 4
#2	#VF29696	Video recorder F	date 5
…	…	…	
#65432	#VA1236	Video recorder A	date 16965

Phone calls table

Inter ref.	Date	Time	Duration
#P1564	date 1	07:32:45 (UTC-4)	00:02:13
#P65465	date 1	07:32:46 (UTC-4)	00:13:24
#P1564	…	…	…
#P455	date 2	08:13:34 (UTC-2)	00:06:56
#P1564	date 2	08:13:35 (UTC-4)	00:34:28
#P654369	date 2	08:13:35 (UTC-4)	01:27:45
…	…	…	…
#P65432	date n	22:56:12 (UTC-2)	00:12:52

Internet connections table

VideoRec.	Date	Name	Mb	…	…
#MG3685	date 1	07:32:45 (UTC-4)	42	…	…
#ME1236	date 1	07:32:46 (UTC-4)	8	…	…
#MG3685	…	…	…	…	…
#MF5896	date 2	08:13:34 (UTC-2)	2	…	…
#MB65435	date 2	08:13:35 (UTC-4)	12	…	…
#MG3685	date 2	08:13:35 (UTC-4)	27	…	…
…	…	…	…	…	…
#MH236	date n	22:56:12 (UTC-2)	0.7	…	…

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DATABASE

- Set of tables with relations

Customer table

Customer	Sexe	Age	Adress	City	Paiement mode	Active
#1	M	35	« 34 St. Denis »	Montréal	Interact	yes
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#MB65435	date 2	08:13:35 (UTC-4)	12	...	...
#MG3685	date 2	08:13:35 (UTC-4)	27	...	...
...	...	...	...	...	...
#MH236	date n	22:56:12 (UTC-2)	0.7	...	...

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LARGE SOURCE OF ANALYSES

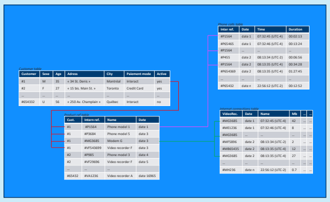

Table of phone calls per customer
Table of Internet connexions per customer
Table of material use per customer / region
Table of customers / region / material ...

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

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CONTENTS

- Essentials of linear and logistic regression models
- Methods for evaluating the performance of predictive models (learning-validation-test data; cross-validation; ROC curve)
- Regression and classification tree
- Random forest
- « Gradient boosting »
- Neural network – Introduction to multilayer perceptron neural networks

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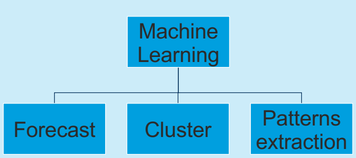
MACHINE LEARNING

- Objectives of ML



	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

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OBJECTIVES 1/3

- **Forecast**
  - Obj : Determine outputs in function of inputs. Outputs = f(inputs).
  - **Supervised** methods: the analyst selects which variables are inputs / outputs.
    - *Discret* outputs : **Classification methods**
    - *Continuous* outputs : **Estimation methods**
  - Different methods : Regressions, decision trees, decision rules, neural networks…

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

	X1	X2	X3	Y1
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C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	2
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

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OBJECTIVES 2/3

- **Cluster**
  - Obj: identify groups of similar objects
  - **Unsupervised** methods
    - Maximize similarity within each group
    - Maximize dissimilarity between groups
  - Different metrics / methods : k-median, hirarchical algorithms, neural networks…

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

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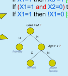
OBJECTIVES 3/3

- **Patterns extraction**
  - Obj: Explain/highlight **relations** existing in the data, **associations** between variables.
  - **Supervised and unsupervised** methods
    - Links analysis :
      - Association rules : A $\Rightarrow$ B (support, confiance)
    - Explanatory models (trees)
    - Visualization : simplify data undertanding.

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

If X1=1 then X3 =1 [5, 3/5]
If (X1=1 and X2=0) then X3=1 [3, 3/3]
If X1=1 then !X1=0 [5, 100%]



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IN BRIEF…

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Forecasting

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	2
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Clustering

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Description

If X1=1 then X3 =1 [5, 3/5]
If (X1=1 and X2=0) then X3=1 [3, 3/3]
If X1=1 then !X1=0 [5, 100%]
…

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MACHINE LEARNING

ML is not a magical tool, ML is not new, ML is not recent. ☺

But the combination of :
- Improved power of computers,
- Large accessible sets of data
- « new » computing methods (use of libraries instead of developing them) and philosophy (code sharing),

Permitted the development of ML by the possible use of (many) past and (some) recent mathematical tools, on large (and cheap) accessible amount of data.

ML considers:
- Statistical tools,
- Data manipulation tools,
- Visualisation tools,
- Neural networks,
- And others

Machine Learning
Supervised → Workshop #3
Unsupervised → Workshop #4

ML considers individual data instead of characteristics of populations

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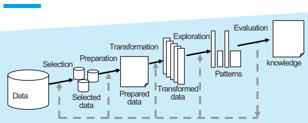
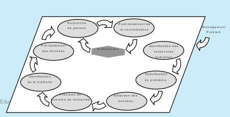
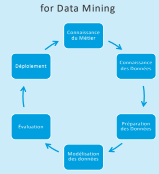
MACHINE LEARNING IS A PROCESS



+



CRISP – DM
Cross Industry Standard Process for Data Mining



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ESSENTIALS OF LINEAR AND LOGISTIC REGRESSION MODELS

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IN BRIEF…

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Forecasting

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
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C4	1	0	1	2
C5	1	0	..	2
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Clustering

	X1	X2	X3	Y1
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Description

If X1=1 then X3 =1 [5, 3/5]
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…

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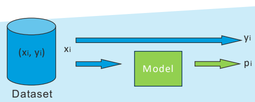
MODELS



	X1	X2	X3	Y1
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C3	1	0	1	2
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Models are dedicated to represent the reality in « something » that can link real observations y_i to conditions x_i.

A model is not reality, it is just a simplified way, eventually comprehensive, we can use to predict what may occur (p_i) in some circumstances (x_i).

If there is a difference between the model predictions (p_i) and what happens in the real data (y_i): the model is wrong, not the real data…

A model may provide predictions p_i that differ to real situation y_i, but if the difference is small enough, we may use it to make predictions.

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LINEAR REGRESSION

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LINEAR REGRESSION

- We have a set of data (x_1, x_2, …x_p) and corresponding output y
- We assume the data follows a model of the following form (linear)

$$y = a_0 + a_1x_1 + a_2x_2 + \ldots + a_px_p + \varepsilon$$

- We compute a_i coefficients that minimise error between real and predicted y
- We evaluate the model performance (which validates or not initial assumption)

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« SIMPLE » LINEAR REGRESSION

- To compute the a_i, the criterion is to minimise the Mean Squared Error

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(p_i - y_i)^2$$

Ex 0 –
Run a first model

Google any function !
See all parameters

- All a_i are supposed “valid” they may be very small
- If 2 (or more) variables are correlated, one may receive most “influence” on a_i

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LASSO REGRESSION

- *Least Absolute Shrinkage and Selection Operator*
- Similar to "simple" linear regression, but, to compute the a_i the criterion is to minimise the Mean Squared Error, under constraint.
- If variables have small influence, they are removed from the model
  - Permits to select un sub-set of « strong » variables, making the model easier to interpret
  - Works if the number of parameters (ai) is smaller that the size of the data set (number of examples)
- But :
  - If some variables are highly correlated and important for the model, Lasso will keep only one and not consider the others

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RIDGE REGRESSION

- Similar to Ridge, but different penality
  - Correlated variables share their relative influence, it is called «shrinkage»
- Rq :
  - x_i have to be centered and reduced (z_i), and y_i have to be centered (and could be reduced)

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ELASTIC-NET

- A mix of Ridge and Lasso
- Proposes a balance between the selection of variables (Lasso) and the shrinkage of correlated variables (Ridge)

Ex 1-
Run Lasso, Ridge and ElasticNet
Compare the models
Change alphas, observe influence
How to select a « good » alpha ?

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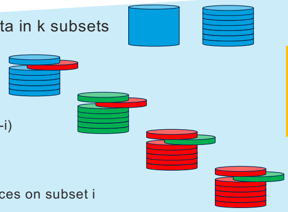
SELECT THE BEST PARAMETER WITH CROSS VALIDATION

- Split the learning data in k subsets
- For i=1 to k
  - Remove subset i
  - Learn on subsets (k-i)
  - Predict for subset i
  - Evaluate performances on subset i
- Keep the parameters from the best iteration



Ex 1- CV
Determine alphas
Compare the models

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Ex 2 -
Load a csv dataset
Learn different prediction models
Set the parameters of the models (alphas)
Compare the models

Ex 2 - CV
Load a csv dataset
Learn different prediction models
Get the best set of parameters (alphas) for the models
Compare the model

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LOGISTIC REGRESSION

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LOGISTIC REGRESSION

Ex 3 -
Classification problem

```
from sklearn.linear_model import LogisticRegression
```

- Similar to linear regression, but for classification
  - We have a set of data (x_1, x_2, …x_p) and corresponding output y
  - We assume the data follows a model of the following form (linear)

$$y = a_0 + a_1x_1 + a_2x_2 + \ldots + a_px_p + \varepsilon$$

- We compute a_i coefficients that minimize misclassifications instead of distance.
- Two steps :
  1. evaluates the probability of being in a given classification
  2. a threshold permits acceptance or rejection of the classification

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METHODS FOR EVALUATING THE PERFORMANCE OF PREDICTIVE MODELS

- *learning-validation-test data*
- *cross-validation*
- *ROC curve*

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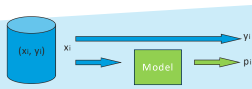
VALIDATION OF ONE PREDICTION



$p_i \approx y_i$?

1. p_i and y_i are numerical values (1, 2, 3, 4.76, -1 120 000)

$$e_i = p_i - y_i$$

2. p_i and y_i are symbolic values (yes/no, red/green/blue)

$$\begin{cases} p_i = y_i \Rightarrow e_i == 0 \\ p_i <> y_i \Rightarrow e_i == 1 \end{cases}$$

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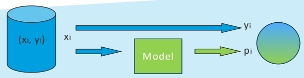
VALIDATION OF A MODEL



We need to evaluate not on one item but on on the dataset

1. r_i and y_i are numerical values (1, 2, 3, 4.76, -1 120 000)

   $e_i = p_i - y_i$, becomes … see next slide

2. r_i and y_i are symbolic values (yes/no, red/green/blue)

   $\begin{cases} p_i = y_i \Rightarrow e_i == 0 \\ p_i <> y_i \Rightarrow e_i == 1 \end{cases}$, becomes … see the following ones ☺

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SOME PERFORMANCE INDICATORS (FOR CONTINUOUS OUTPUTS)

- Mean Error (easy but + vs -)

$$ME = \frac{1}{n}\sum_{i=1}^{n}(p_i - y_i) = \frac{1}{n}\sum_{i=1}^{n} e_i$$

- Mean Square Error (solves + vs – but difficult to explain)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(p_i - y_i)^2 = \frac{1}{n}\sum_{i=1}^{n} {e_i}^2$$

- Root Mean Square Error (solves + vs –, easier to explain, but sensitive to outliers)

$$RMSE = \frac{1}{n}\sqrt{\sum_{i=1}^{n}(p_i - y_i)^2} = \frac{1}{n}\sqrt{\sum_{i=1}^{n} {e_i}^2}$$

- Mean Absolute Error (solves + vs –, easier to explain, robust to outliers)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|p_i - y_i| = \frac{1}{n}\sum_{i=1}^{n}|e_i|$$

- Mean absolute percentage error (solves + vs –, easier to explain, robust to outliers)

$$MAPE = \frac{1}{n}\sum_{i=1}^{n}\frac{|p_i - y_i|}{r_i} = \frac{1}{n}\sum_{i=1}^{n}\frac{|e_i|}{r_i}$$

Ex 4 -
```
from sklearn.metrics import mean_squared_error
from sklearn.metrics import mean_absolute_error

y_true = [3, -0.5, 2, 7]
y_pred = [2.5, 0.0, 2, 8]

mean_squared_error(y_true, y_pred)
mean_absolute_error(y_true, y_pred)
```

With :
- *r_i real value for i*
- *y_i predicted value for i*
- *e_i prediction error for i*
- *n number of predictions*

Those are just examples, the good metric depends on the problem to solve. Instead on mean errors we may have :

- Cumulative errors
- Mean or cumulated weighted errors
- Mean or cumulated thresholds errors
- …

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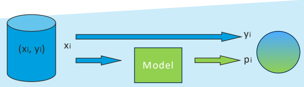
SOME PERFORMANCE INDICATORS (FOR TWO DISCRETE OUTPUTS)



Confusion matrix

		p_i	
		true	false
r_i	true	TP	FN
	false	FP	TN

Accuracy= (TP+TN)/(TP+FN+FP+TN)
Error Rate = (FP+FN)/(TP+FN+FP+TN)=1-Accuracy

True Positive Rate (=sensitivity=recall) = TP/(TP+FN)
False Positive Rate = FP/(FP+TN)

Precision = TP/(TP+FP)

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SOME PERFORMANCE INDICATORS (FOR TWO DISCRETE OUTPUTS)

Confusion matrix

y_i \ p_i	true	false
true	TP	FN
false	FP	TN

Accuracy= (TP+TN)/(TP+FN+FP+TN)

Error Rate = (FP+FN)/(TP+FN+FP+TN)=1-Accuracy

True Positive Rate (=sensitivity=recall) = TP/(TP+FN)

False Positive Rate = FP/(FP+TN)

Precision = TP/(TP+FP)

Ex 5 –

```
y_true  = [0, 1, 1, 1, 1, 1, 0, 0]
y_pred = [0, 0, 1, 1, 1, 1, 1, 1]

from sklearn.metrics import confusion_matrix
confusion_matrix(y_true, y_pred)

from sklearn.metrics import accuracy_score
accuracy_score(y_true, y_pred)
5/8

from sklearn.metrics import precision_score
precision_score(y_true, y_pred, average=None)
1/2
4/6

from sklearn.metrics import recall_score
recall_score(y_true, y_pred, average=None)
1/3
4/5
```


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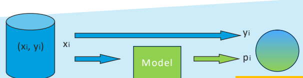
SOME PERFORMANCE INDICATORS (FOR MORE THAN TWO DISCRETE OUTPUTS)



y_i \ p_i	p	o	x	Sum
p	2	0	0	2
o	2	0	0	2
x	1	0	0	1
Sum	5	0	0	5

Accuracy= ( )/( )

Error Rate = (+)/( )

True Positive Rate, for p = $\square$ /

Precision, for p = $\square$ /

Ex 6 -

```
y_true = [1, 2, 3, 1, 2, 2, 1, 2, 3]
y_pred = [1, 1, 3, 1, 2, 3, 1, 2, 3]

from sklearn.metrics import confusion_matrix
confusion_matrix(y_true, y_pred)

from sklearn.metrics import accuracy_score
accuracy_score(y_true, y_pred)

from sklearn.metrics import precision_score
precision_score(y_true, y_pred, average=None)

from sklearn.metrics import recall_score
recall_score(y_true, y_pred, average=None)
```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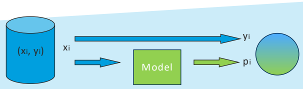
ROC CURVE, AUC



y_i \ p_i	true	false
true	TP	FN
false	FP	TN

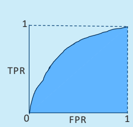
True Positive Rate = TP/(TP+FN)
False Positive Rate = FP/(FP+TN)

When evaluating if an object x_i should be classified true or false, statistical classifiers evaluate a « probability » s to be true and compare it to a threshold (S) :

- If s >= S, the classification is « valid » and returns true
- If s < S, the classification is « unvalid » and returns false

varying s from 0 to 1 gives ROC (receiver operating characteristic) curve

AUC=area under the curve



Ex 7 -
Learning performance
ROC and AUC

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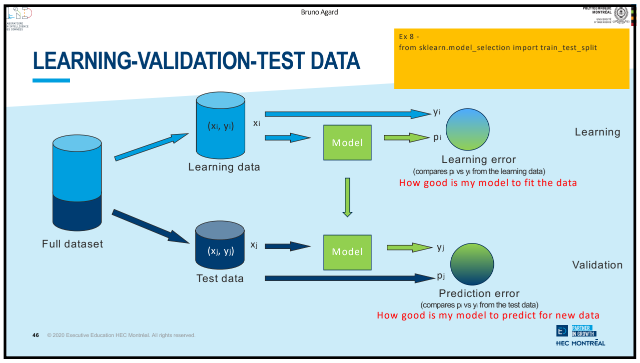
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LEARNING-VALIDATION-TEST DATA
Ex 8 -
from sklearn.model_selection import train_test_split
Full dataset
(xi, yi)
Learning data
xi
Model
yi
pi
Learning
Learning error
(compares pi vs yi from the learning data)
How good is my model to fit the data
(xj, yj)
Test data
xj
Model
yj
pj
Validation
Prediction error
(compares pj vs yj from the test data)
How good is my model to predict for new data
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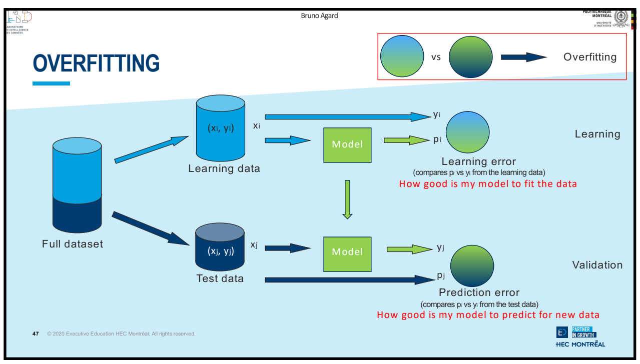
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OVERFITTING
vs
Overfitting
Full dataset
(xi, yi)
Learning data
xi
Model
yi
pi
Learning
Learning error
(compares pi vs yi from the learning data)
How good is my model to fit the data
(xj, yj)
Test data
xj
Model
yj
pj
Validation
Prediction error
(compares pj vs yj from the test data)
How good is my model to predict for new data
47
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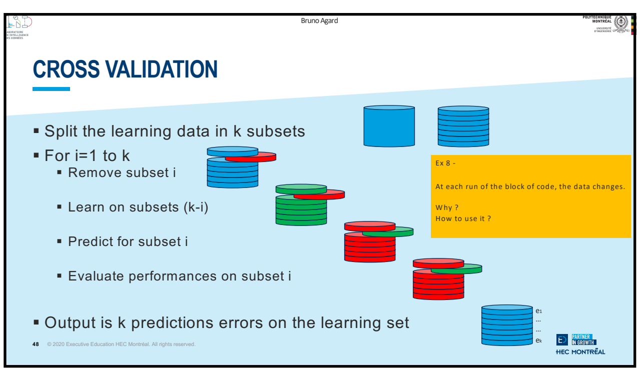
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CROSS VALIDATION
▪ Split the learning data in k subsets
▪ For i=1 to k
▪ Remove subset i
▪ Learn on subsets (k-i)
▪ Predict for subset i
▪ Evaluate performances on subset i
▪ Output is k predictions errors on the learning set
Ex 8 -
At each run of the block of code, the data changes.
Why ?
How to use it ?
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CROSS VALIDATION

Ex 9 - Logistic regression

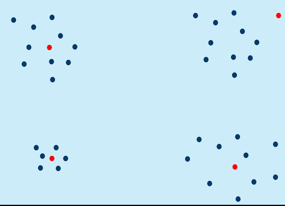
Ex 10 - Linear regressions

- Simply compute
  - Mean error

$$E = \frac{1}{k}\sum_{i=1}^{k} e_i$$

  - Error dispersion

$$\sigma^2 = \frac{1}{k}\sum_{i=1}^{k} (e_i - E)^2$$



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BOOTSTRAP

- Similar to cross validation, but
  - Subsets are built by a random selection of items (x_i, y_i) with replacement
    - A same item (x_i, y_i) may appear more than once on the k subsets
    - Another item (x_i, y_i) may never appear in any subset

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TREES

- *Regression and classification trees*
- *Random Forest*
- *Gradiant Boosting*

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IN BRIEF…

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Forecasting

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	2
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Clustering

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Description

If X1=1 then X3 =1 [5, 3/5]
If (X1=1 and X2=0) then X3=1 [3, 3/3]
If X1=1 then !X1=0 [5, 100%]
…

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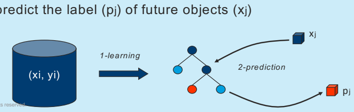
DECISION TREES

- A decision tree allows to classify records (x_i, y_i), by hierarchical division of the whole dataset into subclasses focusing on grouping together items with similar labels (y_i).
- The tree
  - is built from a set of learning objects (x_i, y_i) for which we already know the labels (y_i),
  - will be used to predict the label (p_j) of future objects (x_j)



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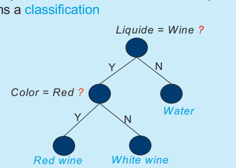
CHARACTERISTICS OF A DECISION TREE

- A decision tree is composed of nodes, branches and leaves :
  - Each node tests an attribute
  - Each branch corresponds to the value of an attribute (in response to the test)
  - Each leaft performs a classification



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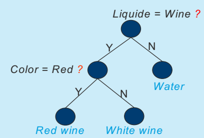
DECISION TREE

- A decision tree can naturally be translated into deduction rules.



- Rules:
  - If Liquide ≠ Wine then Water
  - If (Liquide = Wine and Color = Red) then Red wine
  - If (Liquide = Wine and Color ≠ Red) then White wine

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BUILDING A DECISION TREE

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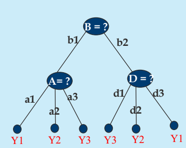
TREE PARAMETERS

	A	B	...	K	Y
C1	a1	b2	...	k4	Y1
C2	a3	b1	...	k8	Y2
...	...	...	...	...	...
Ci	a2	b2	...	k3	Y1
...	...	...	...	...	...
Cn	a3	b1	...	k1	Y3

- Objectives:
  - Classify objects in homogeneous classes
  - Cover all the data

- Questions:
  - How to chose the attributes (A, B, …K) ?
  - How to isolate discriminant values (a1, a2 …) ?



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CONSTRUCTION PROCEDURE

- The tree starts at a node P representing all the data
- Partition(P)
  - If all objects are homogeneous, then the node becomes a leaf, labeled with the name of the class.
  - Otherwise, partition the data according to the most discriminating attribute
    - for each attribute A
      - evaluate the quality of partitioning according to A
    - use the best partitioning to divide P into P1, P2, ...Pn
    - for i = 1 to n do Partition(Pi);

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OBSERVATIONS

- The process is recursive
- Recursivity stops when:
  - The objects assigned to a class are homogeneous
  - There are no more attributes for dividing
  - There is no object with the attribute value
- Problem:
  - how to define the "best" partitioning

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EVALUATE THE QUALITY OF A PARTITIONING

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SELECTION OF THE PARTITIONNING ATTRIBUTE

- When partitionning, is it better to select A, B, …K ?
- For each attribute (A, B, …K)
  - Partition according the selected attribute,
  - Evaluate the partition
- Select the best attribute

	A	B	…	K	Y
C1	a1	b2	…	k4	Y1
C2	a3	b1	…	k8	Y2
…	…	…	…	…	…
Ci	a2	b2	…	k3	Y1
…	…	…	…	…	…
Cn	a3	b1	…	k1	Y3

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EVALUATE A PARTITIONNING

- The quality of a partitioning differs according to the algorithm :
- The goal is to gain a maximum of information at each partition.
  - Minimizes « disorder » in each class
- Different measures of disorder:
  - Continuous output: based on dispersion (statistical variance)
    Regression tree
  - Discrete output: based on misclassification (Impurity index, Gini index, Entropy,..)
    Classification tree

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CONTINUOUS OUTPUT

- Compute variance within each partition P_J

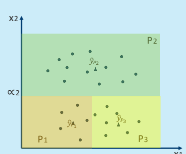
$$V_{P_j} = \frac{1}{|P_J|}\sum_{i \in P_j}\left(y_i - \hat{y}_{P_j}\right)^2$$

- add the variances, weighted by the size of the groups

$$D = |P_J|\sum_{j=i}^{J} V_{P_J}$$

- Or directly

$$D = \sum_{j=i}^{J}\sum_{i \in P_j}\left(y_i - \hat{y}_{P_j}\right)^2$$



- A good score is when all y_i within P_j are close to $\hat{y}_{P_j}$, then D is close to 0

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DISCRETE OUTPUTS

- The purpose of the indicator is to give a note to a partition
- A partition receives a:
  - good score if all elements in the partition are homogeneous (100% yes or 100% no)
  - bad score if all the elements are mixed (50% yes and 50% no)
- Indicators are based on the proportion of individuals of each type in each class.
  - So, in fact, we measure the degree of mixing

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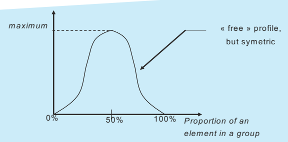
DEGREE OF MIXING



- Gini index
- Entropy
- Others…

- Criterion: For all attributes (A, B …K), the division of node j is performed using the variable that ensures the maximum reduction of misclassifications

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GINI INDEX

- Gini index of a partition p
  - gini(p) = $1 - \sum_i p_i^2$
  - p_i = relative frequency of class i in partition p (% of i in p)
  - Criterion : minimizing gini(p)

ENTROPY

- Entropie of a partition p
  - E(p) = $-\sum p_i \log(p_i)$
  - p_i = relative frequency of class i in partition p
    - Gain = E(before division) - $\sum_j \propto_j$ * E(each resulting partition)
    - $\propto_j$ is the proportion of individuals in each son j
  - Criterion: maximizing gain of entropy

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SIMPLE EXAMPLE

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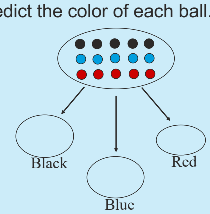
EXAMPLE: OBJECTIVE

- The goal is to classify balls according to attributes X[0], X[1], X[2], so as to be able to predict the color of each ball.

X[0]	X[1]	X[2]	y
1	2	2	Black
2	1	2	Blue
1	1	1	Red
1	2	2	Red
1	2	2	Red
1	1	2	Black
2	1	2	Blue
1	2	2	Black
2	2	2	Blue
2	2	1	Red
1	1	2	Black
2	2	2	Blue
2	1	2	Blue
2	2	2	Black
1	2	1	Red



Proportion	C1
Black	0,33
Blue	0,33
Red	0,33
Gini	0,66666667

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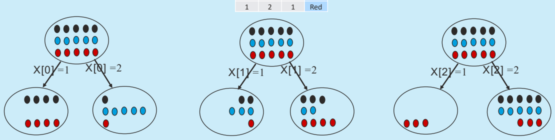
ALTERNATIVES

X[0]	X[1]	X[2]	y
1	2	2	Black
2	1	2	Blue
1	1	1	Red
1	2	2	Red
1	2	2	Red
1	1	2	Black
2	1	2	Blue
1	2	2	Black
2	2	2	Blue
2	2	1	Red
1	1	2	Black
2	2	2	Blue
2	1	2	Blue
2	2	2	Black
1	2	1	Red



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EXAMPLE : ATTRIBUTE X[0]

Ex 20 –

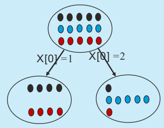
X=X0
max_depth=1

- Gini index of a segment s :
  - i(s) = $1 - \sum_i p_i^2$
  - p_i is the proportion of individuals of class i in s.
- Entropy of a segment s :
  - E(s) = $-\sum_i p_i \log(p_i)$

$1 - \sum_i p_i^2$

Proportion	C1	C2	Sigma
Black	0,50	0,14	
Blue	0,00	0,71	
Red	0,50	0,14	
Gini	0,5	0,44897959	0,476

$\sum_j P_j * i(N_j)$



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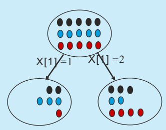
EXAMPLE : ATTRIBUTE X[1]

Ex 20 –

X=X1
max_depth=1

Proportion	C1	C2	Sigma
Black	0,33	0,33	
Blue	0,50	0,22	
Red	0,17	0,44	
Gini	0,61111111	0,64197531	0,589



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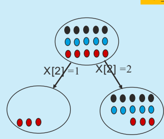
EXAMPLE : ATTRIBUTE X[2]

Ex 20 –

X=X2
max_depth=1

Proportion	C1	C2	Sigma
Black	0,00	0,42	
Blue	0,00	0,42	
Red	1,00	0,17	
Gini	0	0,625	0,500



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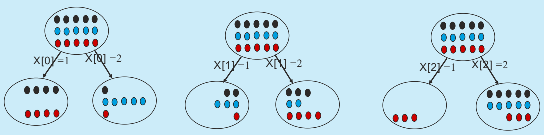
CHOICE



Criterion	X[0]	X[1]	X[2]
Gini	0,476	0,589	0,5

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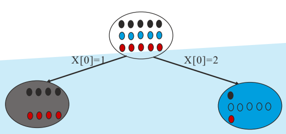
STEP 1



Accuracy : 00 %		Predictions		
		Black	Blue	Red
Real	Black	4	1	0
	Blue	0	5	0
	Red	4	1	0

Ex 20 –

X=X0+X1+X2
max_depth=1

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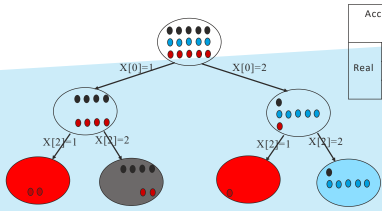
STEP 2



Accuracy : 80 %		Predictions		
		Black	Blue	Red
Real	Black	4	1	0
	Blue	0	5	0
	Red	2	0	3

Ex 20 –

X=X0+X1+X2
max_depth=2

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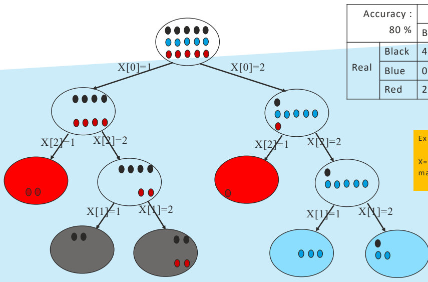
STEP 3



Accuracy : 80 %		Predictions		
		Black	Blue	Red
Real	Black	4	1	0
	Blue	0	5	0
	Red	2	0	3

Ex 20 –

X=X0+X1+X2
max_depth=3

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PRUNING

- Trees that are too bushy are useless
  - Interest of pruning to simplify the tree
- Possibility to apply it on the whole data set or on a subset reserved for validation
- Can be applied
  - during creation of the tree
  - After creation of the tree
- Examples of pruning criteria:
  - partitioning to be deleted if :
    - Gain < threshold

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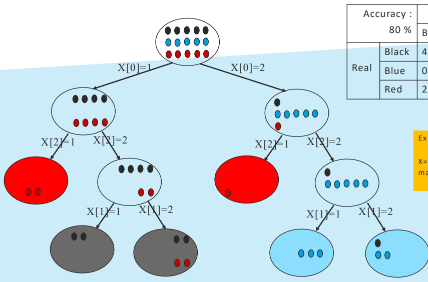
STEP 3



Accuracy : 80 %		Predictions		
		Black	Blue	Red
Real	Black	4	1	0
	Blue	0	5	0
	Red	2	0	3

Ex 20 –

X=X0+X1+X2
max_depth=3

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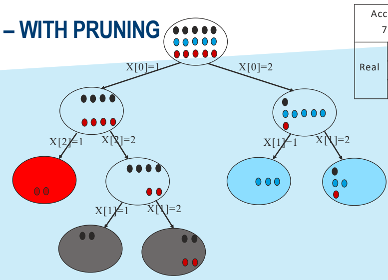
STEP 3 – WITH PRUNING



Accuracy : 73.33 %		Predictions		
		Black	Blue	Red
Real	Black	4	1	0
	Blue	0	5	0
	Red	2	1	2

Ex 20 –

X=X0+X1+X2
max_depth=3
min_samples_leaf=2

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« DIFFERENT » ALGORITHMS

Name	Criterion	Features	Missing values	Pruning	
ID3	Information gain ($\Delta Entropy$)	Discrete	no	no	Classification Binary trees (yes/no)
CART	Gini	Discrete Continuous	yes	yes	Classification and regressions Binary trees (yes/no)
C4.5	Gain ratio ($\frac{\Delta Entropy}{Entropy}$)	Discrete Continuous	yes	yes	Classification and regressions Full trees (yes/no)
C5.5	Gain ratio ($\frac{\Delta Entropy}{Entropy}$)	Discrete Continuous	yes	yes	Applies a boosting method on C4.5

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LARGE DATABASES

- Previous algorithms assume that the data is stored in memory.
- Easily parallelizable methods
  - SPRINT (VLDB96 -- J. Shafer et al.'96)
  - Scalable PaRallelizable INndution of decision Tree
  - Does not require a resident structure in memory
  - Parallel scaled version

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DATA STRUCTURE (ATTRIBUTE LISTS)

Age	Car Type	Risk
23	family	High
17	sports	High
43	sports	High
68	family	Low
32	truck	Low
20	family	High

Age	Class	rid
17	High	1
20	High	5
23	High	0
32	Low	4
43	High	2
68	Low	3

Car Type	Class	rid
family	High	0
sports	High	1
sports	High	2
family	Low	3
truck	Low	4
family	High	5

Figure 3: Example of attribute lists

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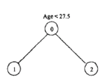
EVOLUTION DES LISTES

Attribute lists for node 0

Age	Class	Tid
17	High	1
20	High	5
23	High	0
32	Low	4
43	High	2
68	Low	3

Car Type	Class	Tid
family	High	0
sports	High	1
sports	High	2
family	Low	3
truck	Low	4
family	High	5



Attribute lists for node 1

Age	Class	Tid
17	High	1
20	High	5
23	High	0

Car Type	Class	Tid
family	High	0
sports	High	1
family	High	5

Attribute lists for node 2

Age	Class	Tid
32	Low	4
43	High	2
68	Low	3

Car Type	Class	Tid
sports	High	2
family	Low	3
truck	Low	4

Figure 4: Splitting a node's attribute lists

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Ex 21 -
Classification tree

See influence of parameters

Learning error / prediction error
(misclassifications)

Ex 22 -
See the differences with classification trees

See influence of parameters

Learning error / prediction error
(distances)

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RANDOM FOREST

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RANDOM FOREST

To make a random forest of n trees from base B :

1. Split base B in n subsets
   - Sample n observations (lines) with draw and put back
   - Sample p variables (columns) with and put back (p is about √(number of variables))
2. On each subset, a decision tree is trained
3. You get n trees... that you keep.
4. The prediction of the random forest is the result from simple majority vote from all n trees.

- Advantage: parallel computation, less sensitive to unbalancing, smaller trees, easy to implement, improves the performance of the chosen tree technique, excellent for VERY large problems (compared to other methods)
- Disadvantage: you lose the visual aspect of unique decision trees.

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	3
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Ex 23 -

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GRADIENT BOOSTING

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GRADIENT BOOSTING

- Boosting methods are similar to random forest in the way it uses multiple models instead of a unique one.

- All n items (i) receive the same weight (1/n)
- for j=1 to J,
  - A model (j) is learn
  - Each item (i) is tested, and a weighted error rate is computed for (i)
  - Update the weight of each item (i) according to a gradient of the error

- Gives more weight to bad predicted items so as to better consider them in the next model

Ex 24 – Classifier

Ex 25 – Regressor

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NEURAL NETWORK

- *Introduction to multilayer perceptron neural networks*

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IN BRIEF…

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Forecasting

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	2
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Clustering

	X1	X2	X3	Y1
C1	1	0	1	2
C2	1	1	0	3
C3	1	0	1	2
C4	1	0	1	..
C5	1	0	..	2
C6	..	1	0	3
C7	1	1	0	4

Description

If X1=1 then X3 =1 [5, 3/5]
If (X1=1 and X2=0) then X3=1 [3, 3/3]
If X1=1 then !X1=0 [5, 100%]
…

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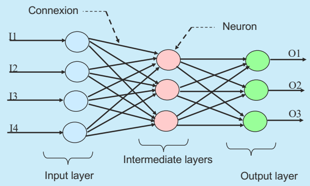
INTRODUCTION

- Neural networks mimic brains, learning process, bla bla bla ☺



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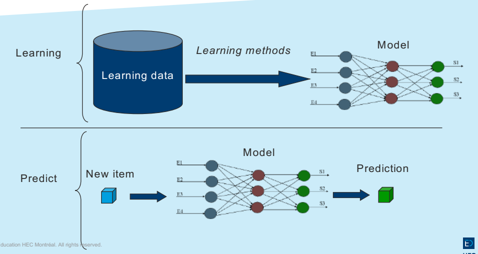
PRINCIPLE



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NEURAL NETWORKS

- Complex networks of elementary, interconnected computing units (neurons).
- A neural network is entirely characterized by
  - its architecture
  - the state transition functions of the neurons.
- Different types of elementary cells
  - Binary or integer values
  - Deterministic or probabilistic output
- Different network architectures
  - With or without feedback (a cell may or may not influence its input)
  - Total or partial feedback
- Different dynamics in the network
  - Synchronous (all cells evolve at the same time)
  - Asynchronous (sequential, random)

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APPLICATIONS

- Learning
  - Supervised
  - Unsupervised
- Learning methods can be:
  - Offline (the entire learning base is processed simultaneously)
  - Online (learning examples are processed one by one when they arrive)

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APPLICATIONS

- Pattern recognition
- Classification
- Prediction
- Vision
- Robotics
- Adaptive control
- For data analysis, the perceptron and the multilayer perceptron are most popular.
  - They are the most "equipped" models
    - Learning Models
    - Learning algorithms
    - Mathematical Evidence

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PERCEPTRON

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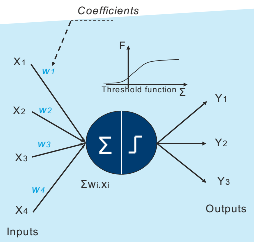
DESIGN



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PERCEPTRON

- The perceptron is a neuron model with a learning algorithm created by Frank Rosenblatt in 1958.
- We will see here the simplified version developed by F. Denis and R. Gilleron.

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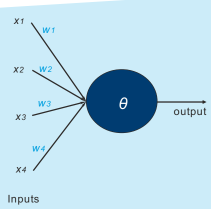
DESCRIPTION



$$Y = \begin{cases} 1, \text{ If } \sum_i x_i . w_i > \theta \\ 0 \text{ , else} \end{cases}$$

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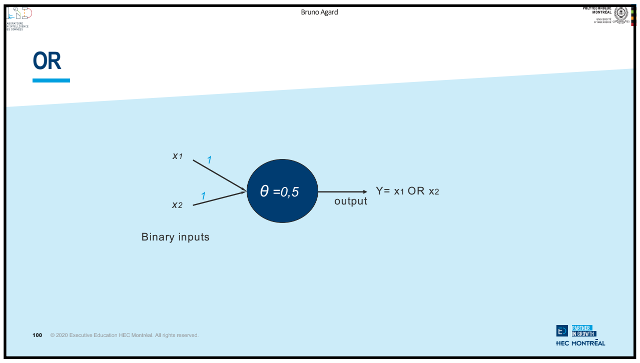

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OR
x1
1
x2
1
θ =0,5
output
Y= x1 OR x2
Binary inputs
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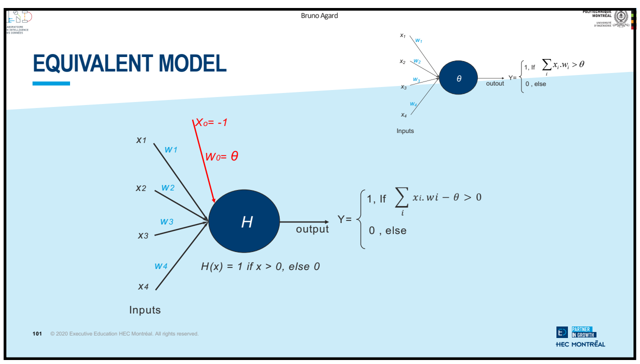

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EQUIVALENT MODEL
X0= -1
W0= θ
x1
w1
x2
w2
w3
x3
w4
x4
H
output
Y=
1, If $\sum_i x_i . w_i - \theta > 0$
0 , else
H(x) = 1 if x > 0, else 0
Inputs
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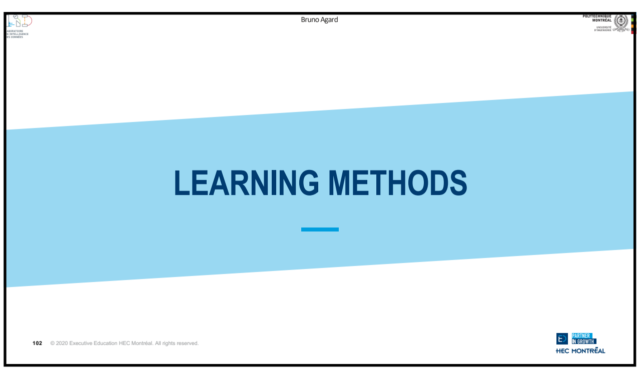

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LEARNING METHODS
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MAIN PRINCIPLE

- Discovery of complex models with progressive refinement
- Classic learning process
  - Initialization of weights w_i to random values
  - Repeat, until stop criterion
    - Presentation of an example
    - Signal propagation in the network
    - Error calculation and weights adjustments
- The network adapts during the learning phase
- Several possible algorithms for weights adjustments

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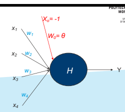
ERROR CORRECTION ALGORITHM



- Inputs :
  - a learning dataset D
  - Random initialization of weights w_i for i between 0 and n
- Repeat, until stop criterion
  - Take an example (s, c) in D
  - Calculate the output o of the perceptron for input s
  - For i from 0 to n - - Updating the weights - - -
    - $w_i = w_i + (c-o).x_i$
- Output :
  - A perceptron P defined by (w_0, w_1, ..., w_n)

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EXEMPLE: APPRENTISSAGE DU OU

étape	w_0	w_1	w_2	Entrée	$\Sigma_0^2 w_i x_i$	o	c	w_0	w_1	w_2
init								0	1	-1
1	0	1	-1	100	0	0	0	0+0x1	1+0x0	-1+0x0
2	0	1	-1	101	-1	0	1	0+1x1	1+1x 0	-1+1x1
3	1	1	0	110	2	1	1	1	1	0
4	1	1	0	111	2	1	1	1	1	0
5	1	1	0	100	1	1	0	1+(-1)x1	1+(-1)x0	0+(-1)x0
6	0	1	0	101	0	0	1	0+1x1	1+1x0	0+1x1
7	1	1	1	110	2	1	1	1	1	1
8	1	1	1	111	3	1	1	1	1	1
9	1	1	1	100	1	1	0	1+(-1)x1	1+(-1)x0	1 +(-1)x0
10	0	1	1	101	1	1	1	0	1	1

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LIMITES

- May not converge
- We don't known if the result will be robust (a new element may differ and reopen gaps)
- No noise tolerance (if an initial, learning information is misfiled, the algorithm will never converge)

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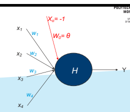
WIDROW-HOFF ALGORITHM



- Inputs :
  - a dataset D
  - Step value $e \in [0 ; 1]$
  - Random initialization of weights w_i for i between 0 and n
- Repeat, until stop criterion
  - Take an example (s, c) in D
  - Calculate the output o of the perceptron for input s
  - For i from 0 to n - - Updating the weights - - -
    - $w_i = w_i + e.(c-o).x_i$
- Output :
  - A perceptron P defined by $(w_0, w_1, \ldots, w_n)$

Ex 30 -

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GRADIENT DESCENT ALGORITHM

- Rather than considering a perceptron that sould correctly classifies each sample one by one, we will consider the error globally on a subset of data.

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GRADIENT DESCENT ALGORITHM

- Inputs :
  - a dataset D, split in subsets S_j
  - Step value $e \in [0 ; 1]$
  - Random initialization of weights w_i for i between 0 and n
- Repeat, until stop criterion
  - For all i, $\Delta w_i = 0$
  - For all samples (s, c) in S
    - Calculate the output o of the perceptron for input s
    - Pour tout i, $\Delta w_i = \Delta w_i + e.(c - o)\, x_i$
  - For i de 1 to n - - Updating the weights - -
    - $w_i = w_i + \Delta w_i$
- Output :
  - Un perceptron P défini par (w_1, ..., w_n)

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MULTI-LAYER PERCEPTRON

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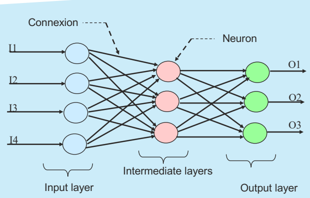
MULTI-LAYER PERCEPTRON



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WHY MULTI-LAYERS ?

- Only one neuron:
  - Limited possibilities, only one calculation, only one operator.
- Several interconnected neurons:
  - More flexibility
  - More possibilities
  - More modeling power

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TOPOLOGY

- Choice of the number of layers
  - inputs, 1 or more hidden layers, outputs
- Choice of the number of neurons per layer
  - depends on inputs and outputs
  - intermediate hidden layers
- Input variables
  - Discrete values
  - Reduced and centered continuous variable [-1,+1].
- Outputs
  - Continuous (estimations)
  - Discrete (classifications)

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DESIGN OF AN MULTI-LAYER PERCEPTRON

- To be able to use multi-layer networks in learning, two things are essential:
  - a method indicating how to choose a network architecture to solve a given problem.
    - how many hidden layers?
    - how many neurons per hidden layer?
- once the architecture is chosen, a learning algorithm that calculates, from the learning samples, the values of the coefficients w_{ij} to build a network adapted to the problem.

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HOW

- For the architecture: auto-constructive algorithms. Research is still very active in this domain. Their role is twofold:
  - learning the sample with a current network,
  - modification of the current network, by adding/deleting new neurons or a new layer, in case of learning failure.
- For learning:
  - Corrections methods.

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EXTENTION OF WIDROW-HOFF ALGORITHM FOR MULTI-LAYERS PERCEPTRONS (SIMPLIFIED)

- Inputs :
  - a dataset D
  - Step value e $\in [0 ; 1]$
  - Random initialization of weights w_i for i between 0 and n
- Repeat, until stop criterion
  - Take an example (s, c) in D
  - Calculate the output o of the perceptron for input s
    - Error on the output d=(c-o)
  - For each layer (from the last, to the first)
    - For neuron i in the layer

$$d_i = o_i(1-o_i) \sum_{k \in succ(i)} d_k w_{ki}$$

  - For all i, j, - - Updating the weights - - -
    - $w_{ij} = w_{ij} + e.d_i.x_{ij}$
- Output :
  - A multi-layers perceptron defined by initial structure and all w_{ij}

Ex 31 -

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SATISFACTION SURVEY

Please take five minutes to complete the **satisfaction survey**.

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THANK YOU!
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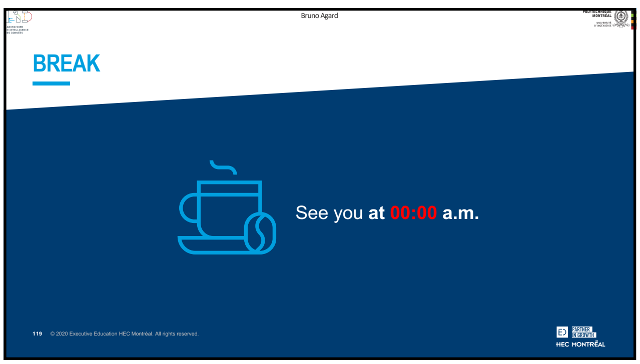
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BREAK
See you at 00:00 a.m.
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