Lecture 4: Supervised learning

Introduction to Machine Learning

Sophie Robert

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Reminders on previous session

Question

Can anyone remind me of the definition of supervised learning ?
Can anyone give me some kind of problems that can be solved with supervised learning ?

This session is **hard but fundamental**: read it slowly and carefully, it is very important in order to understand the rest of the course.

Context

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In this course, we will study **supervised learning**: **we are looking for a function that maps input vectors to labels based on example input-output pairs**.

We will only be focusing on discrete problems, predicting **categorical variables**. Usually, this is referred to as **classification*** problems.

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- Building a set of "examples", consisting of the data describing the individuals (**features***) and the corresponding label (**target***) acting as the **ground truth***
- Building a function mapping this data to this ground truth
- Evaluating the performance of this method either on the example dataset or on some other data (test dataset)

Methodology

Supervised learning methodology

- Represent each individual i by a tuple $(X_i, y_i), X_i \in \mathbb{R}^d, y_i \in \mathcal{Y} = \{1, ..., K\}$
- Define a function f associating each X_i to a label: $f(X_i) \in \mathcal{Y}$

Example

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Features and target

What do you imagine will be some possible features ? will be the target to predict ?

Evaluation

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We need objective metric(s) to assess the quality of the model we designed.

Confusion matrix

Confusion* matrix

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The **confusion matrix** makes it easy to see when the algorithm is "confused".

		Actual	
		Positive	Negative
Predicted	Positive	True Positive	False Positive
	Negative	False Negative	True Negative

Example: compute confusion metric

Build the confusion matrix for the following dataset:

Actual class	Predicted class
0	1
0	0
0	0
0	1
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Question

Can you identify some examples of when you might want to treat false positives / false negatives differently ?

Possible evaluation metrics

Many evaluation metrics rely on the confusion matrix.
Among the most famous:

- **Accuracy***: the proportion of true results among the total number of cases examined.
  $\text{Accuracy} = \frac{TP+TN}{TP+FP+FN+TN}$

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- **Accuracy***: the proportion of true results among the total number of cases examined.
  $\text{Accuracy} = \frac{TP+TN}{TP+FP+FN+TN}$
- **Precision***: the proportion of predicted positives that is truly positive.
  $\text{Precision} = \frac{TP}{TP+FP}$

Possible evaluation metrics

Recall*: the proportion of actual positives correctly classified.
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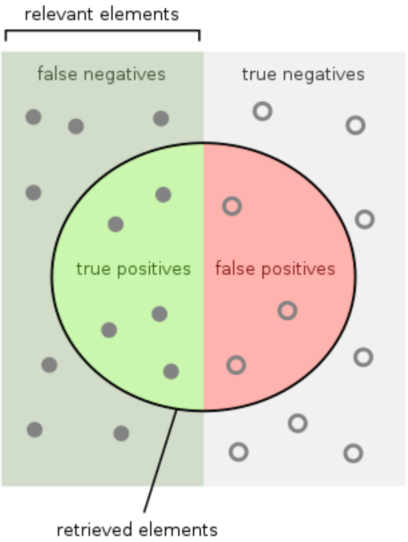
F1-Score*: Harmonic mean of precision and recall.

$F_1 = 2 \times \frac{precision \times recall}{precision + recall}$

Question

Can you identify at least one use-case where you want to favor recall *versus* precision rather than the other ?

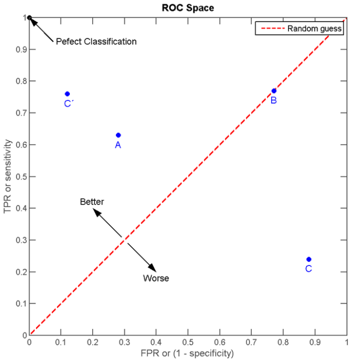
Schematic view of confusion matrix



ROC curve

ROC* curve

ROC curves plots the evolution of the true positive rate and the false negative rate and allows the comparison of models to the random classifier.



ROC curve

Question

For what use-case does the random classifier as a comparison does not work well ?

Example: compute metric value

Using the previous dataset, compute the following metrics:

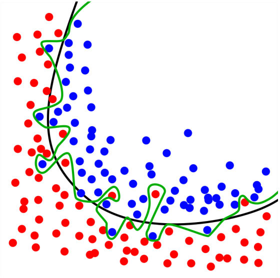
- Accuracy:
- Precision:
- Recall:
- F1-score:

Overfitting

Overfitting*

It is always possible to build a function that will match EXACTLY the training dataset, but it doesn't mean it will generalize well !

It is not always a good idea to have a **perfect fit** for f (i.e, $f(X_i) = y_i$ for all i in the training set).



Bias-variance trade-off

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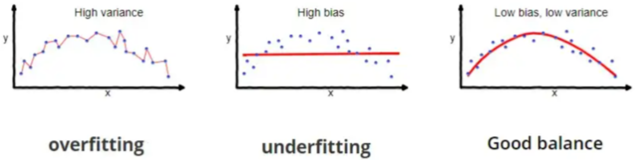
Selecting the right algorithm is a trade-off between **bias*** and **variance***.

- **Bias* error**: error from erroneous assumptions in the learning algorithm (high bias: the algorithm does not learn from the dataset)
- **Variance* error**: error from sensitivity to small fluctuations in the training set (high variance: the algorithm learns the noise from the dataset)



Training / testing dataset

If a 100% fit on the training set is not always the sign of a good model, how can we select the best model ?

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Train and test dataset

We split the dataset into two datasets:

- **Training* dataset**: dataset to build the model
- **Testing* dataset**: dataset to test the model (i.e. compute the scoring metric)

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Question

What issue do you see with this approach ? What should we make sure of when splitting the dataset ?

Cross validation

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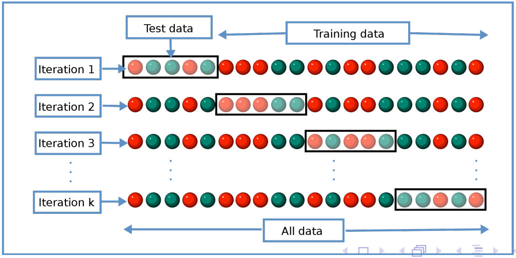

Hyperparameter selection

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A simplistic approach is simply factorial design using k-th cross validation. Other solutions:

- Genetic algorithms
- Simulated annealing
- ...

Beware of overfitting !

Algorithms

Many algorithms are available in the literature ! In this course, we'll study:

- K-nearest neighbors
- Naive Bayes
- Classification trees

Questions

Questions ?