



MACHINE LEARNING

MEI/1

University of Beira Interior,
Department of Informatics

Hugo Pedro Proença,
hugomcp@di.ubi.pt, 2025/2026



Machine Learning

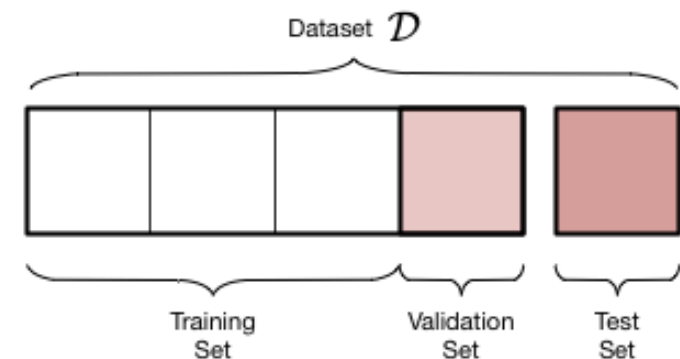
[04]

Syllabus

- Experimental Setup
- Overfitting/Underfitting
 - Regularization
- K-Fold Cross Validation
- Bootstrapping
- Performance Measures
 - Confusion Matrix
 - ROC
 - AUC

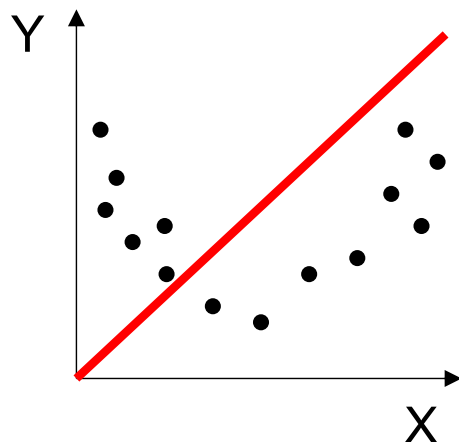
Machine Learning: Experimental Setup

- The design of the experimental procedure to learn/evaluate machine learning models is sensitive
 - Badly designed experiments lead to erroneously **optimistic**/**pessimistic** estimates of the system performance
- One of the golden rules in machine learning is that the data should be split in three disjoint subsets:
 - **Learning (Training) set**: this is the set of instances used to fit the parameters of the hypothesis (model).
 - In case of supervised learning, it consists of pairs of a input vectors and the corresponding ground truth, also known as the target or label.
 - **Validation set**. It provides an unbiased evaluation of a model performance during the learning process, while tuning the model **hyper-parameters** (e.g., acceptance/rejection threshold)
 - **Test set**. It is used to provide an unbiased evaluation of a final model.

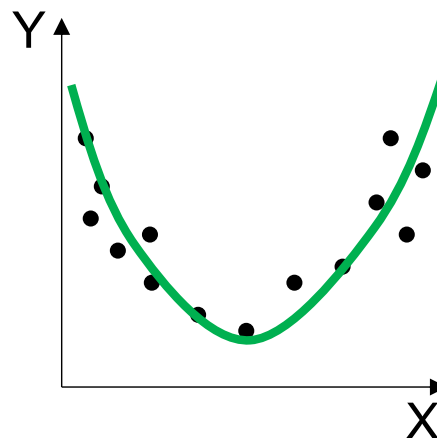


Machine Learning: Overfitting

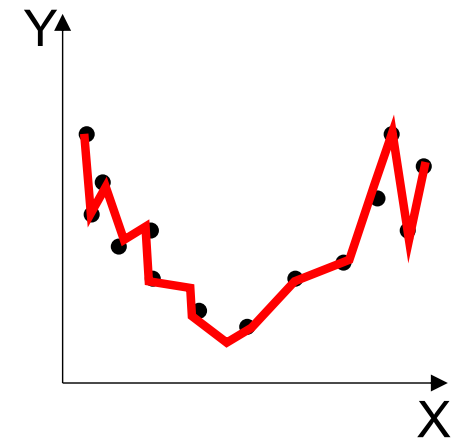
- Overfitting it is one of the most classical problems in Machine Learning problems.
- It occurs when the our model fits “**too well**” the **learning data**, but is **fails to generalize to new data**, i.e., the data where we actually want to use the model
- This is particularly probable when the model has a large number of parameters
 - In such case, the model has too many degrees-of-freedom
 - Nowadays, the breakthrough models based in deep-learning frameworks have a huge number of parameters
 - VGG-16 network, proposed in 2014, has 138,000,000 parameters!



Underfitted



OK



Overfitted

Machine Learning: Overfitting/Underfitting

- The Occam's razzor is a principle from philosophy that states that:
 - »*Entia non sunt multiplicanda praeter necessitatem*»
- This can be translated to:
 - “*More things should not be used than are necessary*”
- Which in practical terms states that simple models should (in case of **comparable effectiveness**) be preferred over more complex ones.



William of Ockham

- In linear and logistic regression, this is equivalent to force the inferred parameters of our model to be small.
- This is done by adding a term to the cost function we want to minimize:
 - It is called the “**regularization term**” (and λ the regularization weight)
 - Consider that $\theta = \{\theta_0, \theta_1, \dots, \theta_D\}$

$$J(\theta) = \frac{1}{2N} \sum_{i=1}^N (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{i=1}^D \theta_i^2$$

Machine Learning: Overfitting/Underfitting

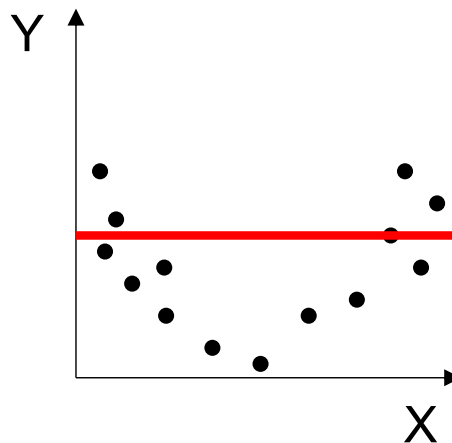
- Consider the following model:

$$h_{\theta}(x) = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4$$

- Suppose that we set λ too large. What happens?
- Minimizing the $J()$ function, it will force that $\theta_1 \dots \theta_4$ will be approximately 0

$$J(\theta) = \frac{1}{2N} \sum_{i=1}^N (h_{\theta}(x^{(i)}) - y^{(i)})^2 + \lambda \sum_{i=1}^D \theta_i^2$$

- Hence, the inferred model will be given by:



**Poor Fitting!!
(Underfitted)**

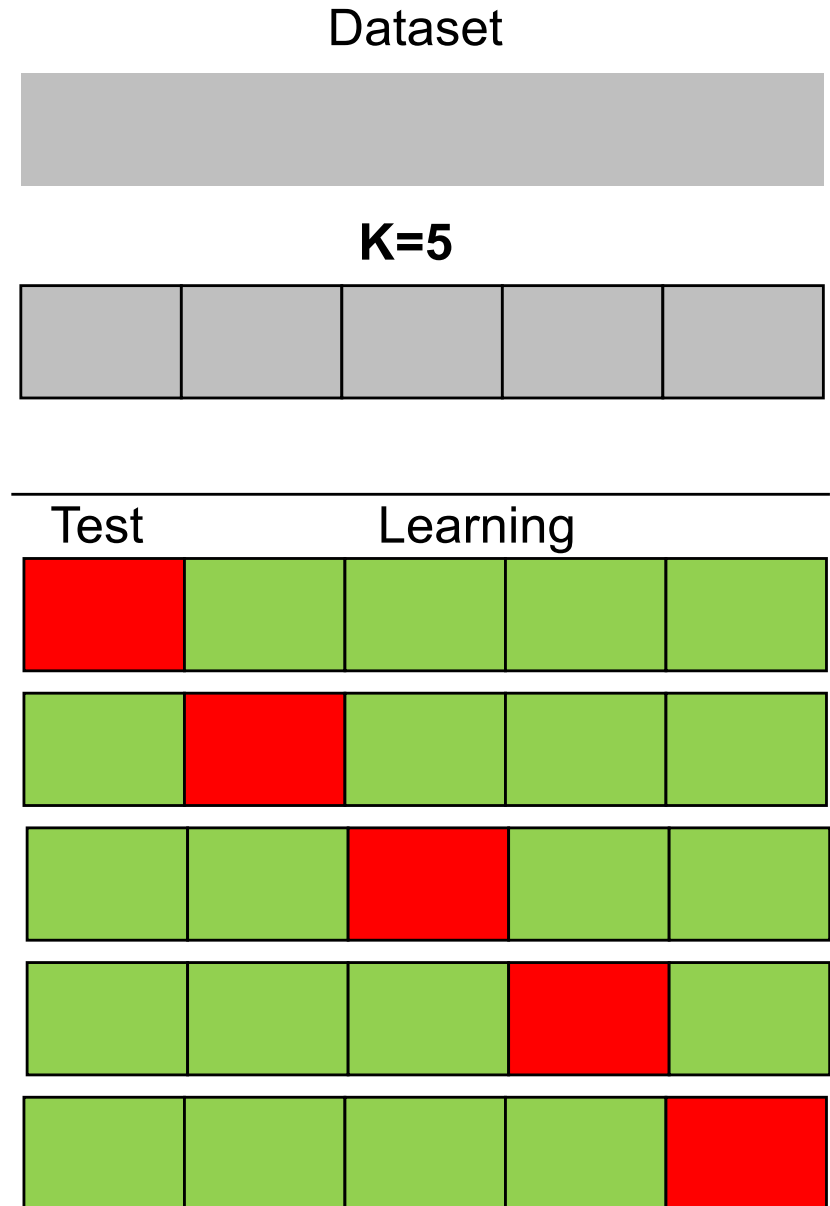
Machine Learning: Overfitting/Underfitting

- In practice terms, this adds one extra-parameter λ to our problem.
 - This parameter is not part of the model, but instead, it is used during the learning process
 - These are called “**hyper-parameters**”
- We saw that:
 - Too large values will lead to **underfitted models**
 - Too small values will lead to **overfitted models**
- Typically, the choice of λ can be made according to the performance in the validation set.
- To adapt the linear and logistic regression learning processes, in order to obtain regularized models, one just have to consider that:

$$\frac{\partial}{\partial \theta_i} \lambda \sum_{i=1}^D \theta_i^2 = 2\lambda \theta_i$$

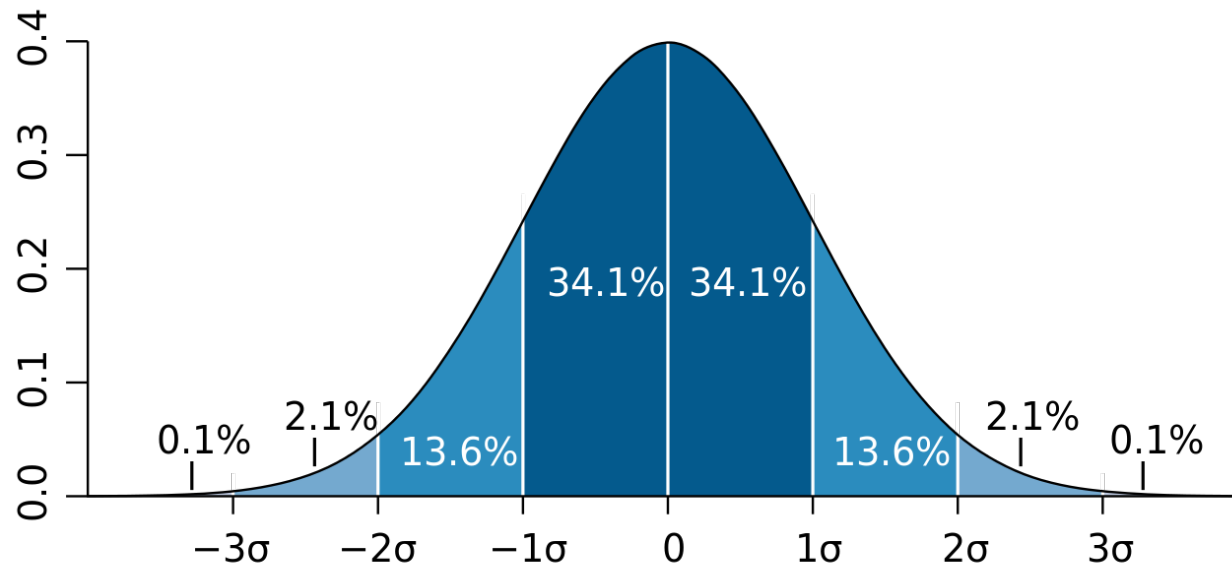
K-Fold Cross Validation

- It is a statistical method used to estimate the performance of machine learning hypotheses (models).
- It is one of the most commonly used, being easy to understand and to implement, with estimates generally having comparable bias than other more sophisticated methods (e.g., bootstrapping)
- It is a **resampling** technique.
 - The value for “K” is defined at the beginning
 - The available data is randomly split at K samples (groups)
 - The model is fitted “K” times, each time using 1 group as **test set** and the remaining (k-1) groups as **learning data**
 - Performance is obtained for the test set
 - The final performance is given by the mean value of the “K” performance values.



K-Fold Cross Validation

- Also, typically results are given in a (“mean” \pm “standard deviation”) performance values
 - E.g.: “0.70 \pm 0.02” means that it is expected that the model performs well 70% of the times, with “typical” variations of more or less 2%
- It has roots in the “**law of big numbers**” and in the “**theorem of the central limit**”
- Considering that repeated observed performance values will approach their “true mean” and that they follow a Gaussian distribution, one can conclude that about 68.2% of the times, the model performance will lie in the “mean \pm standard deviation” interval.



Bootstrapping

- It is closely related to K-fold cross validation and follows the same idea:
 - Generates multiple subsets, by sampling from a single, original dataset.
 - Each of the “*new*” sets can be used to estimate performance.
 - Since there are multiple sets (and therefore multiple estimates), one can also obtain the mean, standard deviation or a confidence interval for the estimate.
- The key difference is that bootstrapping **resamples the data *with replacement***.
 - Given a dataset containing N points, bootstrap picks a data point uniformly at random, adds it to the bootstrapped set, *puts that data point back into the dataset*, and repeats.
 - Why put the data point back?
 - In a real setting, data would come from the “real distribution of the data”.
 - But all we have is a dataset (i.e., a sample), we don’t have the real distribution of the data. Our set is supposed to represent the underlying distribution, i.e., **it is an *empirical distribution of data***.
 - The rule is to simulate sub-sets by drawing from the empirical distribution.
 - Hence, the data point must be put back, because otherwise the empirical distribution would change after each draw.

Confusion Matrix

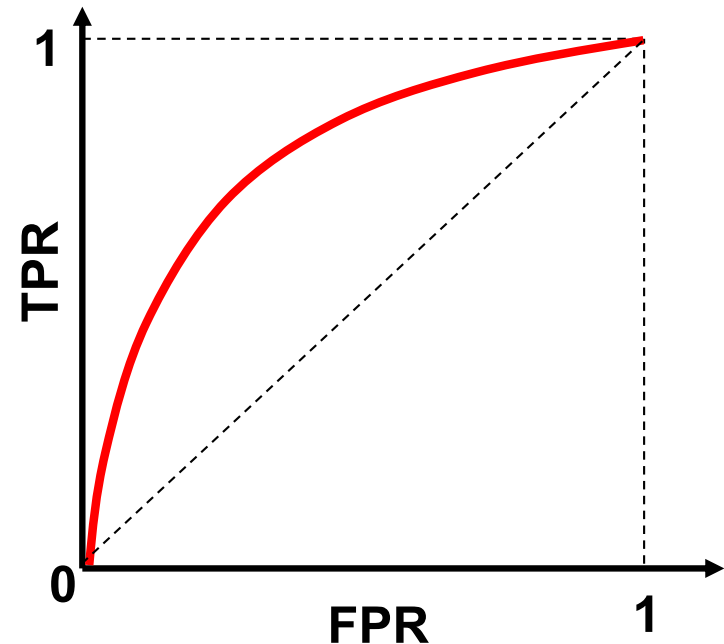
- Also known as an error matrix, this table summarizes the model performance, providing more information than the simple “accuracy” value.
- For a binary classification problem, it is a table with two rows and two columns, reporting the number of *false positives*, *false negatives*, *true positives*, and *true negatives*.
 - Each row corresponds to one predicted outcome (class)
 - Each column corresponds to one actual (ground-truth) class

		Prediction outcome		
		positive	negative	
Actual value	positive	TP	FN	TP + FN
	negative	FP	TN	FP + TN
		TP + FP	FN + TN	

- The model **accuracy** is given by: $\frac{TP+TN}{TP+TN+FP+FN}$
- **Precision:** $\frac{TP}{TP+FP}$ (when it predicts “yes”, how likely it is correct?)
- **Recall:** $\frac{TP}{TP+FN}$ (what is the proportion of “yes” that are actually detected?)

ROC: Receiver Operating Characteristic

- A **Receiver Operating Characteristic curve (ROC)**, is a graphical plot that illustrates the performance of a binary classifier system, with respect to changes in its discrimination threshold.
- This curve shows the relationship between two measures:
 - True Positive Rate
 - False Positive Rate
- The **True Positive Rate (TPR)** is also known as recall and is given by:
 - $TPR = \frac{TP}{TP+FN}$
- The **False Positive Rate (FPR)** ($1 - \text{specificity}$) is given by:
 - $FPR = \frac{FP}{FP+TN}$
- This plot gives the TPR vs. FPR at different acceptance thresholds.
 - Low thresholds classify more items as positive, which increases both the TPR and FPR
 - High thresholds classify less items as positive, which decreases both the TPR and FPR

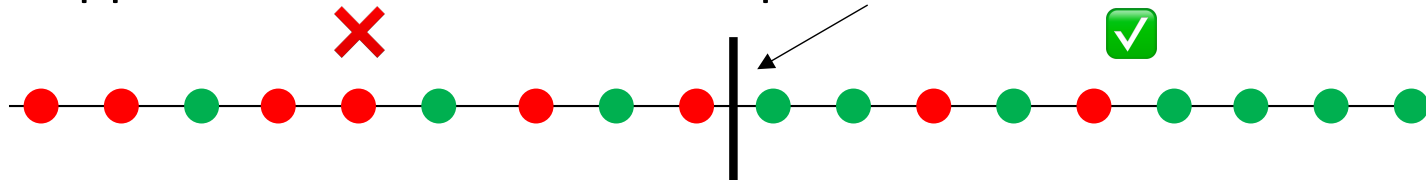


ROC: Receiver Operating Characteristic

- To obtain the data for a ROC curve, we start by sorting the output scores, obtained for the evaluation set:
 - Consider that red dots correspond to class “0” (the *negative* class), and green dots to class “1” (the positive class)



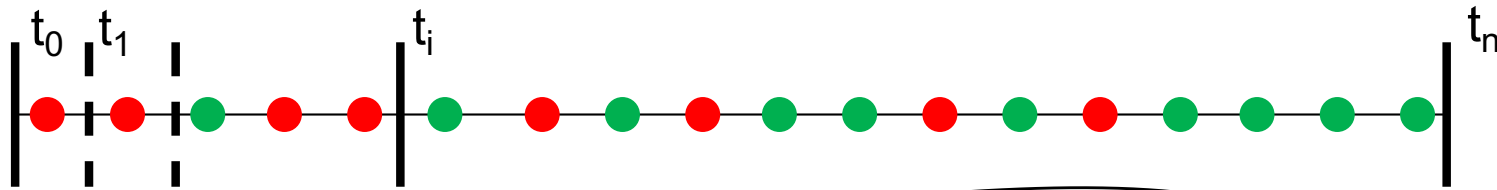
- What happens when we set the acceptance threshold at?



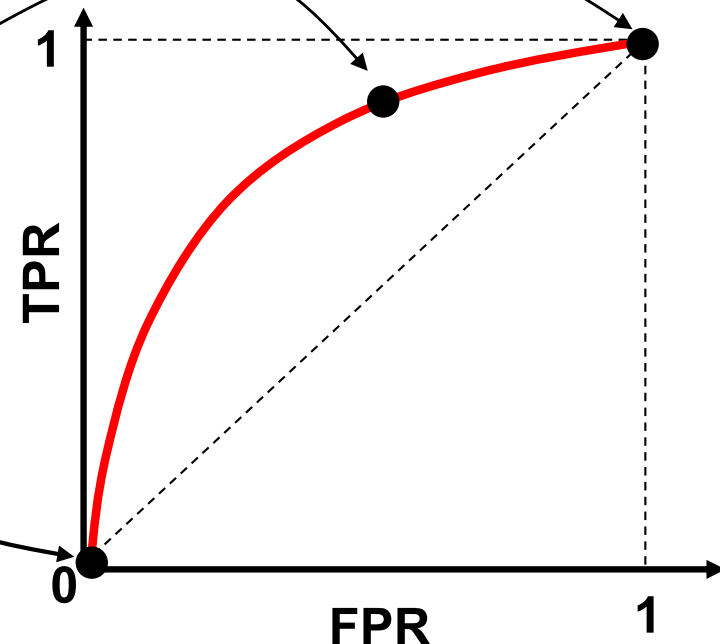
- 6 (out of 8) negative samples are correctly rejected. $TNR=6/8$
- 2 (out of 8) negative samples are erroneously considered as positive. $FPR = 2/8$
- 7 (out of 10) positive samples are correctly accepted. $TPR = 7/10$
- 3 (out of 10) positive samples are erroneously considered as negative. $FNR = 3/10$

ROC: Receiver Operating Characteristic

- Next, we obtain the TPR/FPR values for all possible acceptance thresholds:

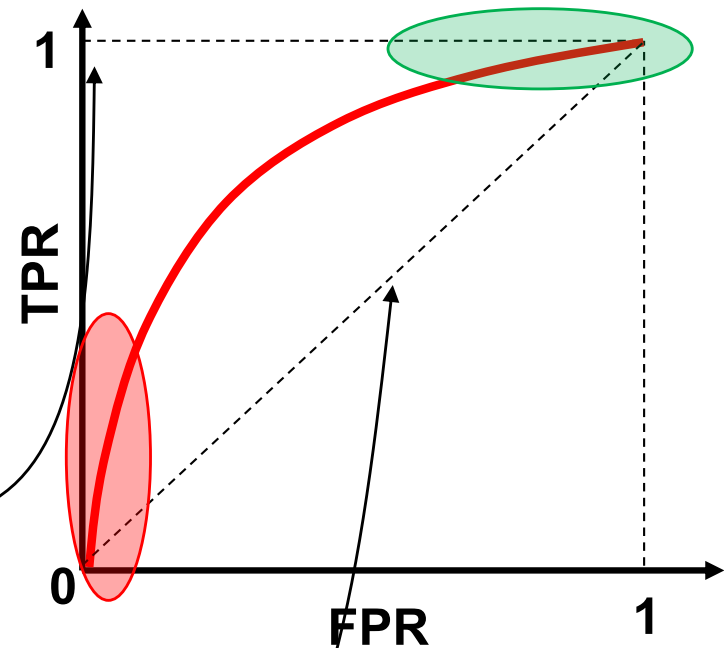


- At t_0 , we have TPR=1, FPR=1
- At t_1 , ...
- At t_i , we have TPR=0.9, FPR=0.5
- ...
- At t_n , we have TPR=0, FPR=0



ROC: Receiver Operating Characteristic

- The ROC curve reports all the possible performance parameterizations of our model:
 - Either tuned for **security** or **convenience**
- When comparing two models, the best one would have the ROC curve above the other most times
- The optimal performance will correspond to the (0,1) point in the plot
- The $x_i=y_i$ line corresponds to the worst possible model, with performance equal of a random number generator.



AUC: Area Under Curve

- The ROC curve shows all possible parameterization, and it is given as a plot
- To obtain a numeric value that summarizes the effectiveness of a model, it is typically used the **Area Under Curve** metric.
- It is given by:
 - $\int_0^1 f(x)dx$
- with $f(x)$ corresponding to the ROC curve values.
- AUC = 1 is the **perfect system** that obtains optimal performance with all possible acceptance thresholds
- AUC = 0.5 is the “random number” generator (**worst possible system**)

