4 Machine Learning Tips and Tricks

4.1 Metrics

Given a set of data points $\{x^{(1)},...,x^{(m)}\}$, where each $x^{(i)}$ has n features, associated to a set of outcomes $\{y^{(1)},...,y^{(m)}\}$, we want to assess a given classifier that learns how to predict y from x.

4.1.1 Classification

In a context of a binary classification, here are the main metrics that are important to track to assess the performance of the model.

❒ **Confusion matrix** – The confusion matrix is used to have a more complete picture when assessing the performance of a model. It is defined as follows:

Actual class \ **Predicted** class	+	–
+	**TP** True Positives	**FN** False Negatives Type II error
–	**FP** False Positives Type I error	**TN** True Negatives

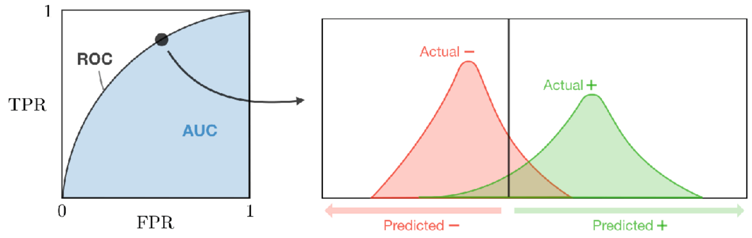
❒ **Main metrics** – The following metrics are commonly used to assess the performance of classification models:

Metric	Formula	Interpretation
Accuracy	$\frac{\text{TP}+\text{TN}}{\text{TP}+\text{TN}+\text{FP}+\text{FN}}$	Overall performance of model
Precision	$\frac{\text{TP}}{\text{TP}+\text{FP}}$	How accurate the positive predictions are
Recall Sensitivity	$\frac{\text{TP}}{\text{TP}+\text{FN}}$	Coverage of actual positive sample
Specificity	$\frac{\text{TN}}{\text{TN}+\text{FP}}$	Coverage of actual negative sample
F1 score	$\frac{2\text{TP}}{2\text{TP}+\text{FP}+\text{FN}}$	Hybrid metric useful for unbalanced classes

❒ **ROC** – The receiver operating curve, also noted ROC, is the plot of TPR versus FPR by varying the threshold. These metrics are are summed up in the table below:

Metric	Formula	Equivalent
True Positive Rate TPR	$\frac{\text{TP}}{\text{TP}+\text{FN}}$	Recall, sensitivity
False Positive Rate FPR	$\frac{\text{FP}}{\text{TN}+\text{FP}}$	1-specificity

❒ **AUC** – The area under the receiving operating curve, also noted AUC or AUROC, is the area below the ROC as shown in the following figure:



4.1.2 Regression

❒ **Basic metrics** – Given a regression model f, the following metrics are commonly used to assess the performance of the model:

Total sum of squares	Explained sum of squares	Residual sum of squares
$\text{SS}_{\text{tot}}=\displaystyle\sum_{i=1}^m(y_i-\overline{y})^2$	$\text{SS}_{\text{reg}}=\displaystyle\sum_{i=1}^m(f(x_i)-\overline{y})^2$	$\text{SS}_{\text{res}}=\displaystyle\sum_{i=1}^m(y_i-f(x_i))^2$

❒ **Coefficient of determination** – The coefficient of determination, often noted R^2 or r^2, provides a measure of how well the observed outcomes are replicated by the model and is defined as follows:

$$\boxed{R^2=1-\frac{\text{SS}_{\text{res}}}{\text{SS}_{\text{tot}}}}$$

❒ **Main metrics** – The following metrics are commonly used to assess the performance of regression models, by taking into account the number of variables n that they take into consideration:

Mallow's Cp	AIC	BIC	Adjusted R^2
$\frac{\text{SS}_{\text{res}}+2(n+1)\widehat{\sigma}^2}{m}$	$2\Big[(n+2)-\log(L)\Big]$	$\log(m)(n+2)-2\log(L)$	$1-\frac{(1-R^2)(m-1)}{m-n-1}$

where L is the likelihood and $\widehat{\sigma}^2$ is an estimate of the variance associated with each response.