Introduction to Machine Learning

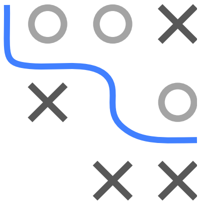
Evaluation
ROC Basics

		True Class y		
		$+$	$-$	
Pred.	$+$	TP	FP	$\text{PPV} = \frac{\text{TP}}{\text{TP}+\text{FP}}$
$\hat{y}$	$-$	FN	TN	$\text{NPV} = \frac{\text{TN}}{\text{FN}+\text{TN}}$
		$\text{TPR} = \frac{\text{TP}}{\text{TP}+\text{FN}}$	$\text{TNR} = \frac{\text{TN}}{\text{FP}+\text{TN}}$	$\text{Accuracy} = \frac{\text{TP}+\text{TN}}{\text{TOTAL}}$

Learning goals

- Understand why accuracy is not an optimal performance measure for imbalanced labels
- Understand the different measures computable from a confusion matrix
- Be aware that each of these measures has a variety of names

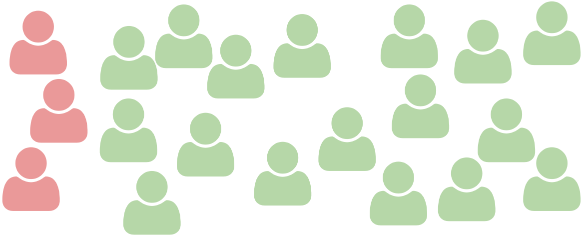
CLASS IMBALANCE

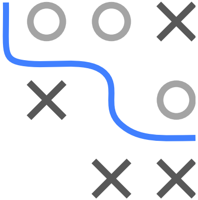


- Assume a binary classifier diagnoses a serious medical condition.
- Label distribution is often **imbalanced**, i.e, not many people have the disease.
- Evaluating on mce is often inappropriate for scenarios with imbalanced labels:
    - Assume that only 0.5 % have the disease.
    - Always predicting “no disease” has an mce of 0.5 %, corresponding to very high accuracy.
    - This sends all sick patients home $\rightarrow$ bad system
- This problem is known as the **accuracy paradox**.

CLASS IMBALANCE / 2

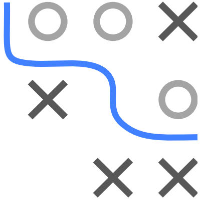
Classifying all observations as “no disease” (green) yields top accuracy simply because the “disease” occurs so rarely → accuracy paradox.





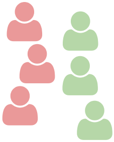
IMBALANCED COSTS

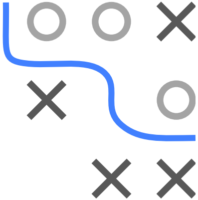
- Another point of view is **imbalanced costs**.
- In our example, classifying a sick patient as healthy should incur a much higher cost than classifying a healthy patient as sick.
- The costs depend a lot on what happens next: we can well assume that our system is some type of screening filter, and often the next step after labeling someone as sick might be a more invasive, expensive, but also more reliable test for the disease.
- Erroneously subjecting someone to this step is undesirable (psychological, economic, medical expense), but sending someone home to get worse or die seems much more so.
- Such situations not only arise under label imbalance, but also when costs differ (even though classes might be balanced).
- We could see this as imbalanced costs of misclassification, rather than imbalanced labels; both situations are tightly connected.



IMBALANCED COSTS / 2

Imbalanced costs: classifying incorrectly as "no disease" incurs very high cost.





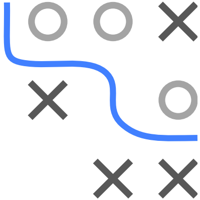
- Problem: if we were able to specify costs precisely, we could evaluate or even optimize on them.
- This important subfield of ML is called **cost-sensitive learning**, which we will not cover in this lecture unit.
- Unfortunately, users find it notoriously hard to come up with precise cost figures in imbalanced scenarios.
- Evaluating "from different perspectives", with multiple metrics, often helps to get a first impression of system quality.

ROC ANALYSIS

- **ROC analysis** is a subfield of ML which studies the evaluation of binary prediction systems.
- ROC stands for “receiver operating characteristics” and was initially developed by electrical engineers and radar engineers during World War II for detecting enemy objects in battlefields – still has the funny name.

`http://media.iwm.org.uk/iwm/mediaLib//39/media-39665/large.jpg`

LABELS: ROC METRICS



From the confusion matrix (binary case), we can calculate "ROC" metrics.

		True Class y		
		$+$	$-$	
Pred.	$+$	TP	FP	$\rho_{PPV} = \frac{\text{TP}}{\text{TP}+\text{FP}}$
$\hat{y}$	$-$	FN	TN	$\rho_{NPV} = \frac{\text{TN}}{\text{FN}+\text{TN}}$
		$\rho_{TPR} = \frac{\text{TP}}{\text{TP}+\text{FN}}$	$\rho_{TNR} = \frac{\text{TN}}{\text{FP}+\text{TN}}$	$\rho_{ACC} = \frac{\text{TP}+\text{TN}}{\text{TOTAL}}$

- True positive rate ρ_{TPR}: how many of the true 1s did we predict as 1?
- True Negative rate ρ_{TNR}: how many of the true 0s did we predict as 0?
- Positive predictive value ρ_{PPV}: if we predict 1, how likely is it a true 1?
- Negative predictive value ρ_{NPV}: if we predict 0, how likely is it a true 0?
- Accuracy ρ_{ACC}: how many instances did we predict correctly?

LABELS: ROC METRICS

Example:

		Actual Class y		
		Positive	Negative	
$\hat{y}$ **Pred.**	Positive	**True Positive** (TP) = 20	**False Positive** (FP) = 180	Positive predictive value = TP / (TP + FP) = 20 / (20 + 180) = **10%**
	Negative	**False Negative** (FN) = 10	**True Negative** (TN) = 1820	Negative predictive value = TN / (FN + TN) = 1820 / (10 + 1820) ≈ **99.5%**
		True Positive Rate = TP / (TP + FN) = 20 / (20 + 10) ≈ **67%**	True Negative Rate = TN / (FP + TN) = 1820 / (180 + 1820) = **91%**	

`https://en.wikipedia.org/wiki/Receiver_operating_characteristic`

MORE METRICS AND ALTERNATIVE TERMINOLOGY

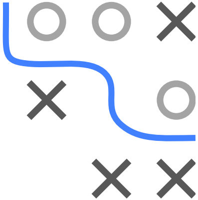
Unfortunately, for many concepts in ROC, 2-3 different terms exist.

		True condition				
	Total population	Condition positive	Condition negative	Prevalence $= \frac{\Sigma \text{ Condition positive}}{\Sigma \text{ Total population}}$	Accuracy (ACC) $= \frac{\Sigma \text{ True positive} + \Sigma \text{ True negative}}{\Sigma \text{ Total population}}$	
Predicted condition	Predicted condition positive	**True positive**, Power	**False positive**, Type I error	Positive predictive value (PPV), Precision $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Predicted condition positive}}$	False discovery rate (FDR) $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Predicted condition positive}}$	
	Predicted condition negative	**False negative**, Type II error	**True negative**	False omission rate (FOR) $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Predicted condition negative}}$	Negative predictive value (NPV) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Predicted condition negative}}$	
		True positive rate (TPR), Recall, Sensitivity, probability of detection $= \frac{\Sigma \text{ True positive}}{\Sigma \text{ Condition positive}}$	False positive rate (FPR), Fall-out, probability of false alarm $= \frac{\Sigma \text{ False positive}}{\Sigma \text{ Condition negative}}$	Positive likelihood ratio (LR+) $= \frac{\text{TPR}}{\text{FPR}}$	Diagnostic odds ratio (DOR) $= \frac{\text{LR+}}{\text{LR−}}$	F_1 score $= \frac{1}{\frac{\frac{1}{\text{Recall}} + \frac{1}{\text{Precision}}}{2}}$
		False negative rate (FNR), Miss rate $= \frac{\Sigma \text{ False negative}}{\Sigma \text{ Condition positive}}$	Specificity (SPC), Selectivity, True negative rate (TNR) $= \frac{\Sigma \text{ True negative}}{\Sigma \text{ Condition negative}}$	Negative likelihood ratio (LR−) $= \frac{\text{FNR}}{\text{TNR}}$		

Clickable version/picture source

Interactive diagram

LABELS: F_1 MEASURE



- It is difficult to achieve high **positive predictive value** and high **true positive rate** simultaneously.
- A classifier predicting more positive will be more sensitive (higher ρ_{TPR}), but it will also tend to give more *false* positives (lower ρ_{TNR}, lower ρ_{PPV}).
- A classifier that predicts more negatives will be more precise (higher ρ_{PPV}), but it will also produce more *false* negatives (lower ρ_{TPR}).

The F_1 **score** balances two conflicting goals:

1. Maximizing positive predictive value
2. Maximizing true positive rate

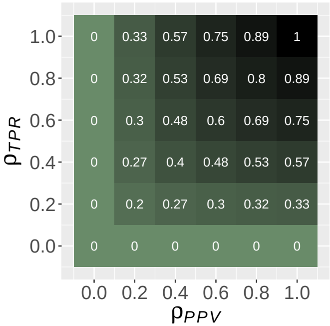
ρ_{F_1} is the harmonic mean of ρ_{PPV} and ρ_{TPR}:

$$\rho_{F_1} = 2 \cdot \frac{\rho_{PPV} \cdot \rho_{TPR}}{\rho_{PPV} + \rho_{TPR}}$$

Note that this measure still does not account for the number of true negatives.

LABELS: F_1 MEASURE / 2

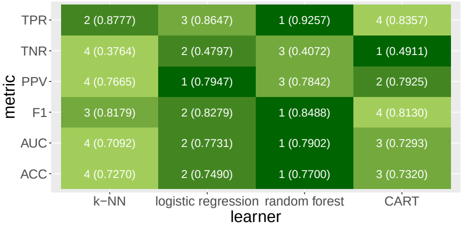
F_1 score for different combinations of ρ_{PPV} & ρ_{TPR}.
$\rightarrow$ Tends more towards the lower of the two combined values.



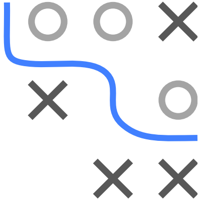
- A model with $\rho_{TPR} = 0$ (no positive instance predicted as positive) or $\rho_{PPV} = 0$ (no true positives among the predicted) has $\rho_{F_1} = 0$.
- Always predicting "negative": $\rho_{F_1} = 0$.
- Always predicting "positive":
  $\rho_{F_1} = 2 \cdot \rho_{PPV}/(\rho_{PPV} + 1) = 2 \cdot n_+/(n_+ + n)$,
  which will be small when the size of the positive class n_+ is small.

WHICH METRIC TO USE?

- As we have seen, there is a plethora of methods.
  $\rightarrow$ This leaves practitioners with the question of which to use.
- Consider a small benchmark study.
  - We let k-NN, logistic regression, a classification tree, and a random forest compete on classifying the `credit risk` data.
  - The data consist of 1000 observations of borrowers' financial situation and their creditworthiness (good/bad) as target.
  - Predicted probabilities are thresholded at 0.5 for the positive class.
  - Depending on the metric we use, learners are ranked differently according to performance (value of respective performance measure in parentheses):



WHICH METRIC TO USE? / 2



- We need not expect overly large discrepancies in general, but neither will we always see an unambiguous picture.
- Different metrics emphasize different aspects of performance.
  $\rightarrow$ The choice should be made in the domain context.
- For practitioners it is vital to understand what should be evaluated exactly, and which measure is appropriate.
  - Regarding credit risk, for instance, defaults are to be avoided, but not at all cost.
  - The bank must undertake a certain risk to remain profitable, so a more balanced measure such as the F_1 score might be in order.
  - On the other hand, a system detecting weapons at an airport should be able to achieve very high true positive rates, even if this comes at the expense of some false alarms.