Title:	Classification - Part II
Course:	Machine Learning
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Master:	Data Science and Business Analytics
Master:	Artificial Intelligence and Innovation
Master:	Finance and Financial Technologies
Academic Year:	2023/2024

Model Selection: Evaluation of a Classifier

Questions to be answered

- Which of the available models for classification is the best one?
- Which of the available algorithms is the best one?
- Which is the best parameters configuration?

$\Longrightarrow$ Evaluation

The Oil Slick example I

- Detect oil slick (failures, illegal dumping) from satellite images, for early alarm
- Radar satellite images
    - Dark regions whose size and shape depend on weather and sea conditions
    - Look–alike dark regions can also be caused by local weather conditions, such as high winds
    - Manual detection by experts is definitely expensive and slow
- Scarcity of training data: oil spills are, fortunately, rare
- Unbalanced nature of data: the negative examples (non–spills) are predominant over the positive ones

The Oil Slick example II

- An automatic hazard detection system has been developed and marketed
    - Pre–selection of images for final manual processing
    - Necessary a tradeoff between undetected spills and false alarms
    - Evaluation of performance guides the tradeoff

The training set

- In supervised learning the training set performance is overoptimistic
- We need a lower bound for performance obtained by independent tests
- Supervised data are usually scarce, we need to balance the use of them between:
  - train
  - validation, to tune the parameter (sometimes it is omitted)
  - test
- Evaluate how much the theory fits the data
- Evaluate the cost generated by prediction errors

Learning and evaluation

- Empirically (and intuitively) the more training data we use the best performance we should expect
    - Statistically, we should expect a larger covering of the situation that can occur when classifying new data
- We must consider the effect of random changes
- The evaluation is independent from the algorithm used to generate the model

The meaning of the *test error*

- let us suppose that the test set is a good representation, *on the average*, of the entire dataset $\mathcal{X}$ (i.e. run–time)
- the relationship between the training set and $\mathcal{X}$ will be subject to probabilistic variability
- the evaluation can be done either at different levels
  - general – the whole performance of the classifier
  - local – the local performance of a component of the model, i.e. a node of a decision tree
- if the test set error ratio is x, we should expect a run–time error $x \pm ???$

$\Rightarrow$ confidence interval

Confidence interval in error estimation

Bernoulli process

- forecasting each element of the test set is like one experiment of a Bernoulli process
    - good prediction $\Rightarrow$ success
    - bad prediction $\Rightarrow$ error
- the same as N independent binary random events of the same type
- $f = S/N =$ empirical frequency of error
- which is p the probability of error?

Empirical frequency and true frequency OPTIONAL

- Deviations of the empirical frequency from the true frequency are due to *noise*
- Usually, noise is assumed to have a normal distribution around the true probability (for $N \geqslant 30$)
- We choose the confidence level, i.e. the probability that the true frequency of success is below the pessimistic frequency that we will compute

$$P\left(z_{\alpha/2} \leqslant \frac{f-p}{\sqrt{p(1-p)/N}} \leqslant z_{1-\alpha/2}\right) = 1-\alpha$$

Range error estimate

OPTIONAL

Wilson score interval

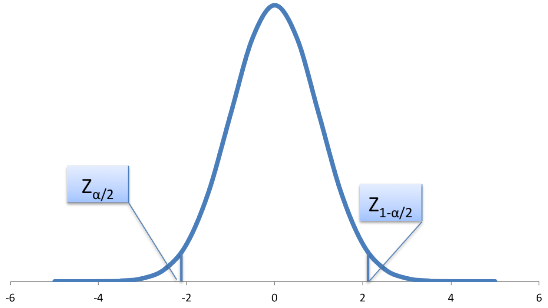
- z depends on the desired confidence level $1 - \alpha$
- it is the abscissa delimiting the area $1 - \alpha$ for a normal distribution
  - i.e. the inverse of the standard cumulative normal distribution
- with a little of algebra

$$\frac{1}{1 + \frac{1}{N} z^2} \left[f + \frac{1}{2N} z^2 \pm z \sqrt{\frac{1}{N} f(1 - f) + \frac{1}{4N^2} z^2} \right]$$

The pessimistic error is obtained by substituting $\pm$ with $+$

Confidence level in error estimation OPTIONAL

The confidence level $1 - \alpha$ is the probability that the estimation of the frequency of good predictions is good, i.e. the probability that the true frequency is inside the confidence interval around the empirical frequency

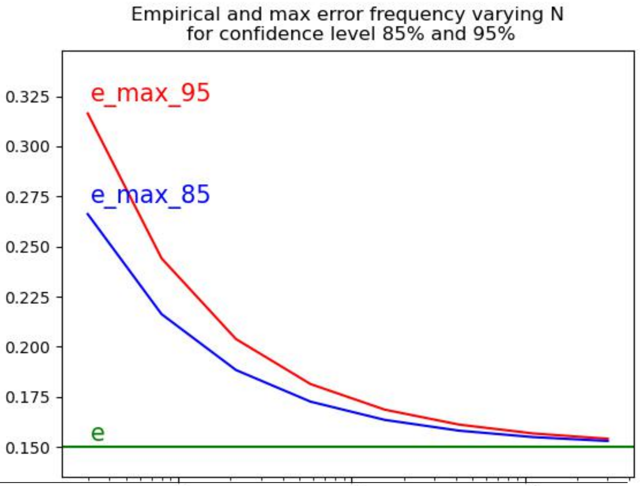


$1-\alpha$	Z
0.99	2.58
0.98	2.33
0.95	1.96
0.90	1.65
0.75	1.04
0.50	0.67

Confidence interval in error estimation OPTIONAL

Increasing N, with constant empirical frequency, the uncertainty for p narrows.

Example:
$f = 85\%$, $\alpha = 0.05$



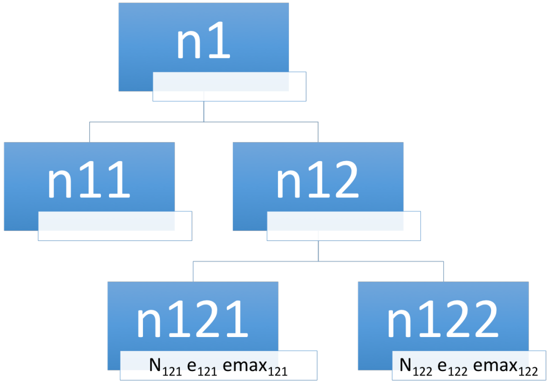
Statistical pruning of DT with error estimation OPTIONAL

The C4.5 strategy

- Consider a subtree near the leaves
- Compute its maximum error e_l as a weighted sum of the maximum error of the leaves
- Compute the maximum error e_r of the root of the subtree transformed into a leaf
- Prune if $e_r \leqslant e_l$
- With pruning, the error frequency increases, but the number of records in node also increases, therefore the maximum error can decrease

DT before pruning

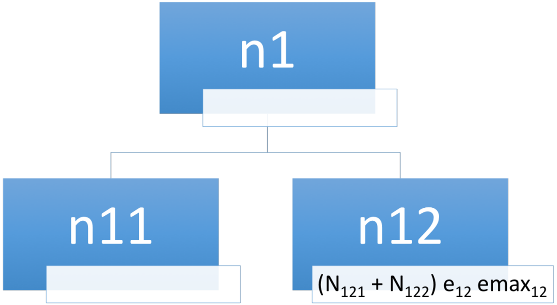
OPTIONAL


n1
n11
n12
n121
N_{121} e_{121} $emax_{121}$
n122
N_{122} e_{122} $emax_{122}$

N_x = Records in node f_x = Error frequency in node e_x = Maximum error frequency in node

DT after pruning

OPTIONAL



$e_x - f_x$ increases as N_x decreases

Pruning is done if $(N_{121} + N_{121}) * e_{12} < N_{121} * e_{121} + N_{122} * e_{122}$

Other pruning techniques - examples

Scikit-Learn allows to adjust pruning with one or more of the hyperparameters below

- **max_depth** - the maximum depth allowed for the tree; it is a *horizontal cut*, pruning all the branches below a given depth
- **min_samples_split** - either the minimum absolute number of samples or the minimum fraction of samples (with respect to the entire population in the dataset) in a node to make a split, if the threshold is not exceeded the node becomes a leaf
- **min_samples_leaf** - the minimum number of samples (or fraction, as above) required to be at a leaf node
- **min_impurity_decrease** - a node will be split if this split induces a decrease of the impurity greater than or equal to this value; if the weighted sum of the descendant leaves do not decrease from the node under consideration more than this threshold then the node becomes a leaf

Accuracy of a classifier

- The error frequency is the simplest indicator of the quality of a classifier
  - it is the sum of errors on any class divided by the number of tested records
- From now on, for simplicity, we will use the empirical error frequencies
  - remember that in real cases the maximum error frequencies should be used instead
- Accuracy and other more sophisticated indicators are used to:
  - compare different classifiers or parameter settings
  - estimate the run–time performance we can expect, and therefore the cost of errors

The *hyperparameters*

Optimizing the model learned

- Every machine learning algorithm has one or more parameters than influence its behaviour
    - they are usually called *hyperparameters*
- Several train/test loops are in general necessary to find the best set of values for the hyperparameters
- It is crucial to obtain a highly reliable estimate of the run–time performance
- Sometimes it is necessary to find the best compromise between the optimisation step and the quality of the result

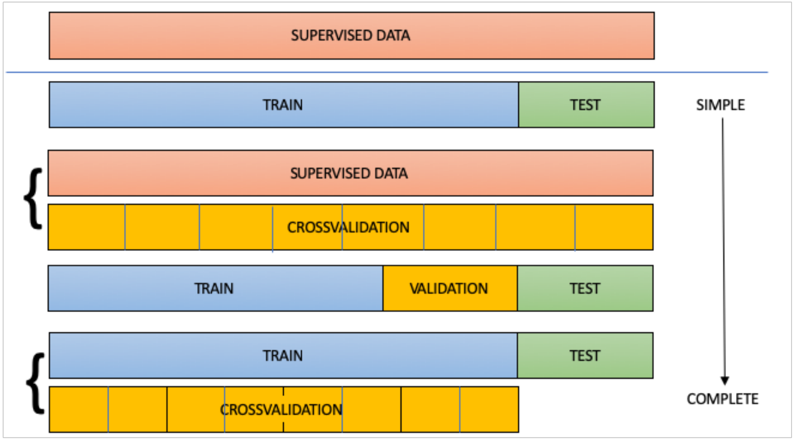
Testing strategies

Getting the most out of the available supervised data

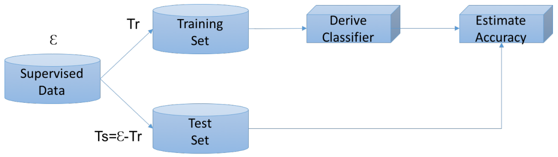
Problem: in every step the data should be *representative* of the data that will be classified run–time

- Holdout
  - splitting data into *training set* and *test set*
  - splitting data into *training set*, *validation set* and *test set*
- Cross validation
  - repeated tests with different splits

The train/test process: some alternatives



Holdout

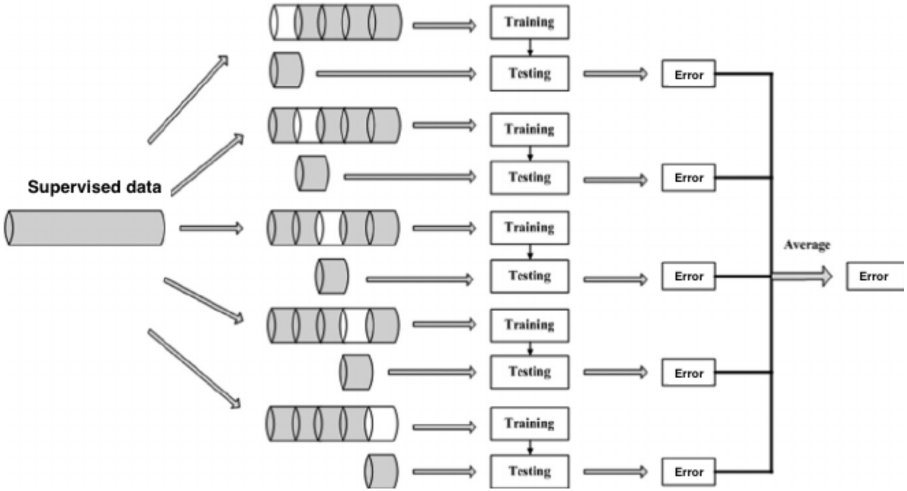


- A typical value of the training/test ratio is 2/1
- The split should be as random as possible
    - It may happen that the proportion of classes in the supervised dataset $\mathcal{X}$ is altered in the Training and Test sets, to prevent such cases the statistical sampling technique of stratification ensures the maintenance of the proportion of classes
- In this setting, the test set is used to obtain an *estimation* of the performance measures with new data

Cross Validation (k–fold)

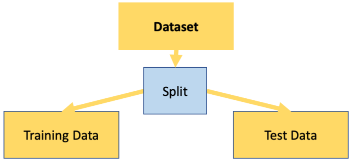
- The training set is randomly partitioned into k subsets
  - If necessary, use stratified partitioning
- k iterations using one of the subsets for test and the others for training
- Combine the result of tests
- Generate the final model using the *entire training set*
- Optimal use of the supervised data
  - each record is used $k-1$ times for training and once for testing
- Typical value: $k = 10$

Cross Validation

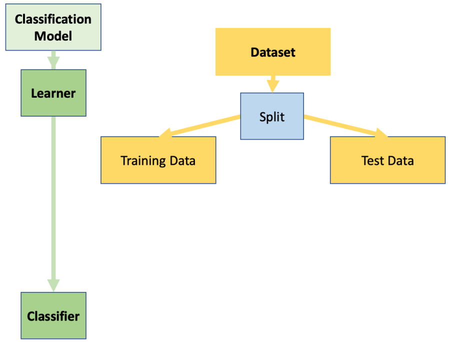


Cross–validation workflow

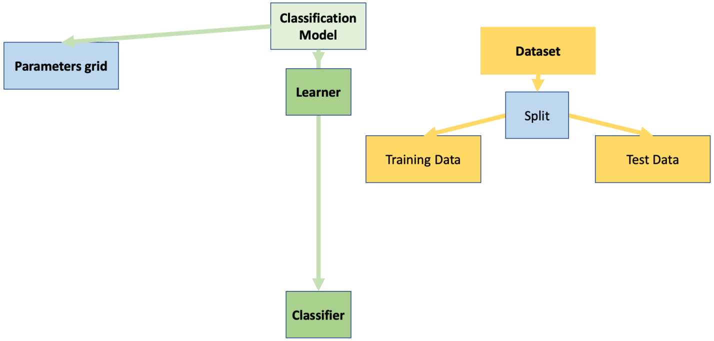
Cross–validation workflow



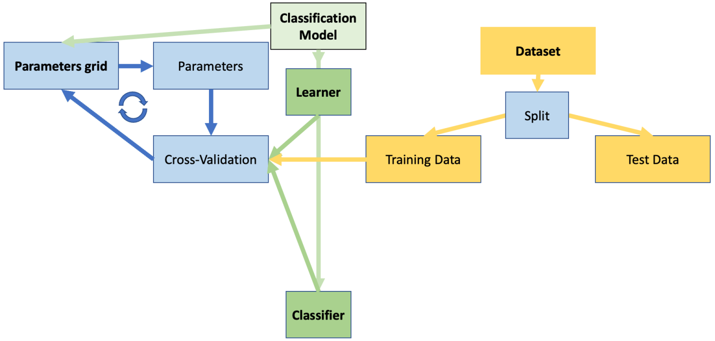
Cross–validation workflow



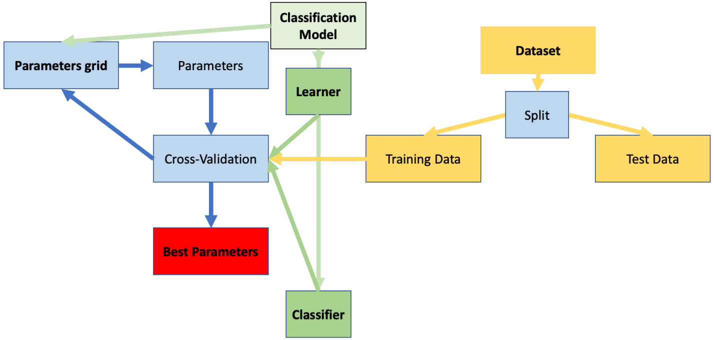
Cross–validation workflow



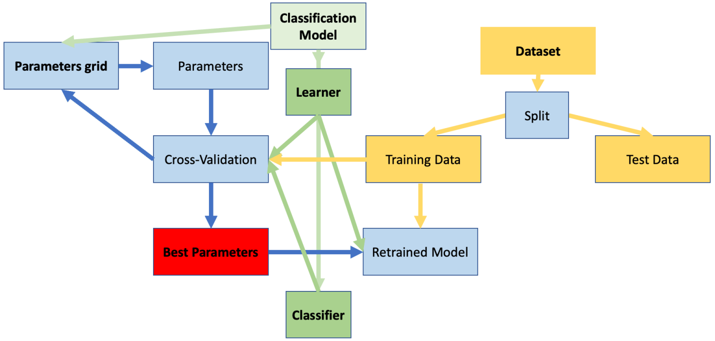
Cross–validation workflow



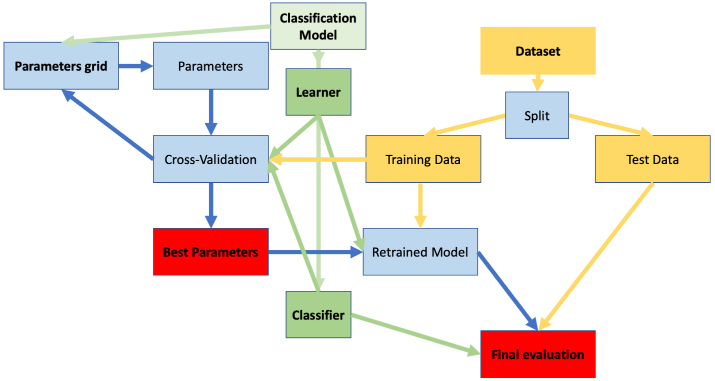
Cross–validation workflow



Cross–validation workflow



Cross–validation workflow



Cross Validation – pros and cons

- ☹ The train/test loop is repeated k times
- ☺ The estimate of the performance is averaged on k runs

  $\Rightarrow$ more reliablity
- ☺ All the examples are used once for testing
- ☺ The final model is obtained using all the examples

  $\Rightarrow$ best use of the examples

Leave one out

Optional

- Extreme case of cross validation, with $k = N$
- No random partitioning
- It is intrinsically non–stratified

Bootstrap

OPTIONAL

- A statistical sampling technique
- Sampling of N records with replacement
  - each record can be selected, even if it has been selected in previous samples
- Some records will never be selected: they will be used for test

$$e = 0.632 e_{test} + 0.368 e_{training}$$

$$\left(1 - \frac{1}{N}\right)^N \approx e^{-1} \approx 0.368$$

Train, Validation, Test – pros and cons OPTIONAL

☺ The train/validation loop is faster than the Cross Validation

☺ The optimisation of the hyperparameters is done with the validation set, independent from the final evaluation

$\Rightarrow$ more reliable than the simple holdout

☹ The test is done on a portion of the examples

$\Rightarrow$ less reliable with respect to Cross Validation

Performance measures of a classifier

Binary prediction

For simplicity: Positive/Negative

- success rate = accuracy

$$\frac{TP + TN}{N_{test}}$$

- error rate

$$1 - \text{success rate}$$

		Predicted class	
		Pos	Neg
True class	Pos	TP	FN
	Neg	FP	TN

Is accuracy enough?

- Is the accuracy the only performance indicator for a classifier? Other possible indicators:
  - Velocity
  - Robustness w.r.t. noise
    - i.e. training data with bad class label
  - Scalability
  - Interpretability
- A classification error can have different consequences, depending on the class of the individual
  - when forecasting an illness a false positive can be less dangerous than a false negative
    - unless the cares or the additional examinations are dangerous or invasive
  - consider the cost of retiring a machinery as damaged, while it is ok (false positive) and the cost of an unpredicted failure (false negative)

A summary of measures I

Precision – $TP/(TP+FP)$
the rate of true positives among the positive classifications

Recall – $TP/(TP+FN)$
the rate of the positives that I can catch (a.k.a. Sensitivity)

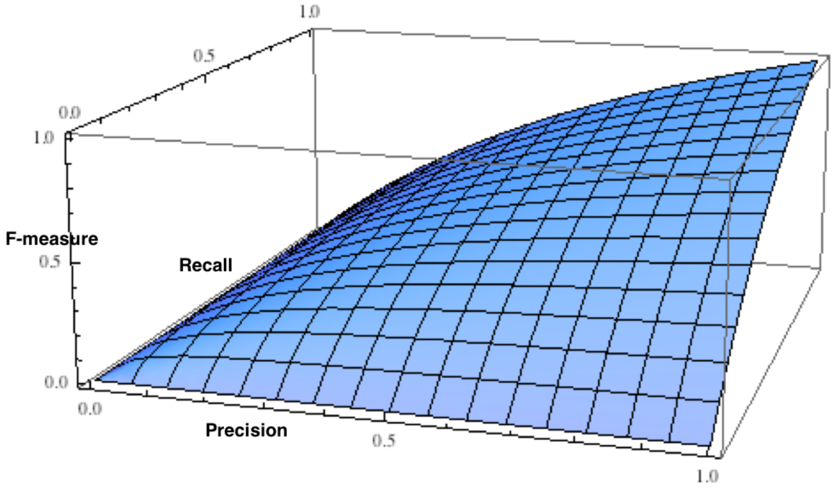
Specificity – $TN/(TN+FP)$
the rate of the negatives that I can catch

A summary of measures II

F1–score – the armonic mean of precision and recall, a.k.a. balanced F-score

$$F = 2\frac{\text{prec} \cdot \text{rec}}{\text{prec} + \text{rec}}$$

F–measure



Which measure should we use?

A rule of thumb

- Accuracy gives an initial feeling of the effectiveness of the classifier, but can be heavily misleading when classes are highly imbalanced
    - it considers globally all the classes, also when $C > 2$ (non-binary case, also called *multi–class*)
- F1–score is *always* interesting, because has higher values when precision and recall are reasonably balanced
- if the the costs of errors on positives and negatives are significantly *different*, then it is *necessary* to evaluate precision and recall.
- for multi–class problems see page 46.

Multi–class case

- The table of page 38 is easily extended and is called confusion matrix
- Each cell contains the number of test records of class i and predicted as class j
- The numbers in the main diagonal are the “true” predictions

Confusion matrix with three classes, say a, b, c

$T_x =$ true number of x labels in the dataset

$P_x =$ total number of x predictions by a given classifier, say $\overline{C}$

$TP_x =$ number of true predictions for class x given by classifier $\overline{C}$

$FP_{i-j} =$ number of false prediction for class i predicted as j

$$\text{accuracy} = \frac{\sum_i TP_i}{N}$$

$$\text{precision}_i = \frac{TP_i}{P_i}$$

$$\text{recall}_i = \frac{TP_i}{T_i}$$

		Predicted class			
		a	b	c	Total
True class	a	TP_a	FP_{a-b}	FP_{a-c}	T_a
	b	FP_{b-a}	TP_b	FP_{b-c}	T_b
	c	FP_{c-a}	FP_{c-b}	TP_c	T_c
	Total	P_a	P_b	P_c	N

Multi-class evaluation I

The number of classes is more than two

- precision, recall and f1–score are intrinsically defined for a single class;
- in binary classification they are commonly referred to the so–called positive class;
- in multi-class cases, the scorers of ‘scikit-learn‘ produce an array of values, one for each class
- when a single value is necessary to optimise the hyper parameters, as in ‘GridSearchCV‘, if we need to maximise one of precision, recall, f1–score an average value is required

Multi-class evaluation II

The number of classes is more than two

averaging of measure f for classes $c_i \in \mathcal{C}$, each class with frequency C_i

- macro average: $f(\mathcal{C}) = \frac{\sum f(c_i)}{C}$
- weighted average: $f(\mathcal{C}) = \frac{\sum f(c_i) * C_i}{C}$
- with macro average the measure of each class has the same impact on the average value, therefore in case of imbalancing the minority classes have influence bigger than their size
- with wighted average the measure of each class influences the result in proportion with its size, therefore in case of imbalancing the minority classes have smaller influence

Beyond pure counting

Taking into account the “a priori” information

- Is it likely to obtain a correct prediction *by chance*?
- Example: early diagnosis
    - let us consider a disease affecting 2% of patients
    - a prediction saying always “no disease” has 98% precision, which, in general would be a good result
    - the evaluation of a prediction should take this as a baseline, and, possibly, look for improvements

Example of confusion matrix

- Confusion matrix of classifier $\overline{C}$ on a given dataset
- 140 correct predictions
- The predicted proportion of classes is 100:60:40

		Predicted class			
		a	b	c	Total
True class	a	88	14	18	120
	b	10	40	10	60
	c	2	6	12	20
	Total	100	60	40	200

Confusion matrix of a random classifier $R_{\overline{C}}$

A *virtual* experiment

- A random classifier $R_{\overline{C}}$ producing the same proportion of classes as $\overline{C}$
  - the horizontal *margin* is the same as $\overline{C}$
- The rows have all the same proportion as the horizontal margin
- 82 predictions are exact by chance
  - the sum of the main diagonal of $R_{\overline{C}}$

		Predicted class			
		a	b	c	Total
True class	a	60	36	24	120
	b	30	18	12	60
	c	10	6	4	20
	Total	100	60	40	200

Taking into account the random component

- The improvement of $\overline{C}$ over $R_{\overline{C}}$ is $140 - 82 = 58$
- The improvement of the perfect classifier is $200 - 82 = 118$
- We define $\kappa(\overline{C})$ the improvement of the classifier at hand w.r.t. the improvement of the perfect classifier

$$\kappa(\overline{C}) = 58/118 = 0.492$$

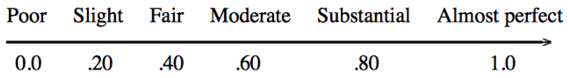
κ statistic[Cohen(1960)]

- Evaluates the concordance between two classifications
  - in our case between the predicted and the true one
- Probability of concordance $\mathbf{Pr}(c) = \frac{TP_a + TP_b + TP_c}{N}$
- Probability of random concordance $\mathbf{Pr}(r) = \frac{T_a * P_a + T_b * P_b + T_c * P_c}{N^2}$
- κ is the ratio between the concordance exceeding the random component and the maximum surplus possible

$$-1 \leqslant \kappa = \frac{\mathbf{Pr}(c) - \mathbf{Pr}(r)}{1 - \mathbf{Pr}(r)} \leqslant 1$$

Range of κ

- 1 for perfect agreement
  - $TP_a + TP_b + TP_c = N$
- -1 for total disagreement
  - $TP_a + TP_b + TP_c = 0$ and there is a perfect swap between predictions and true labels
    - if all classes have non–zero counts -1 is possible only if the number of labels is two
- 0 for random agreement

$\kappa =$ 

The cost of errors

- Our decisions are driven by predictions
- Bad predictions imply a cost
- Examples
    - grant a loan to a person who turns out to be a bad payer costs more than denying a loan to a person that could be a good payer
    - a false “oil spill” alarm is less expensive than an undetected spill
    - a wrong “fault prediction” in an industrial plant is in general less expensive than an unexpected fault disabling the plant and creating damages
    - in direct marketing, sending advertisement material without redemption is less harmful than the loss of business if a promising customer is ignored

Cost sensitive learning I

Weight the errors

- Alternative 1: alterate the proportion of classes in the supervised data, duplicating the examples for which the classification error is higher
  - In this way, the classifier will became more able to classify the classes for which the classification error cost is higher
  - This solution is useful also when the classes are *imbalanced*, that is the frequencies of the class labels in $\mathcal{X}$ are not equal

Cost sensitive learning II

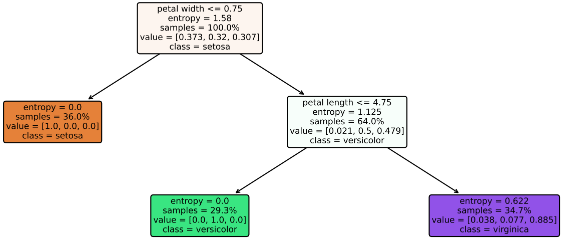
- Alternative 2: some learning schemes allow to add weights to the instances
  - e.g. the `DecisionTreeClassifier` of Scikit-Learn has the hyperparameter **class_weight**: it allows to define a dictionary, with one key per distinct class, specifying the relative weight to be assigned to each class, the optimisation of the fitting will be adjusted accordingly
    - the `balance` option balances the classes automatically

Predicting probabilities of classes I

- Many classifiers produce, rather than a class label (*crisp* prediction), a tuple of probabilities, one for each possible class, (*probabilistic*, or *soft* prediction)
- The adequacy of one output or the other depends on the application domain
    - when an immediate decision is required the crisp output is necessary
    - when the classification is part of a process including several evaluation/action steps the probabilistic output can be more appropriated

Crisp values sometimes hide probabilities

- For example, when a leaf of a decision tree has non–zero counts for the minority classes a less–than–one probability, the probabilities of the examples falling in that leaf can be assigned on the basis of the fractions of the training data elements in that leaf belonging to each class
- Consider the rightmost leaf in the figure (it is the pruned tree of the first module on Classification) [1]



[1] Since it is quite common to have leaves with a small number of examples and/or minority classes with frequencies near to zero, smoothing techniques are used to adjust the probabilities

Probabilities to crisp

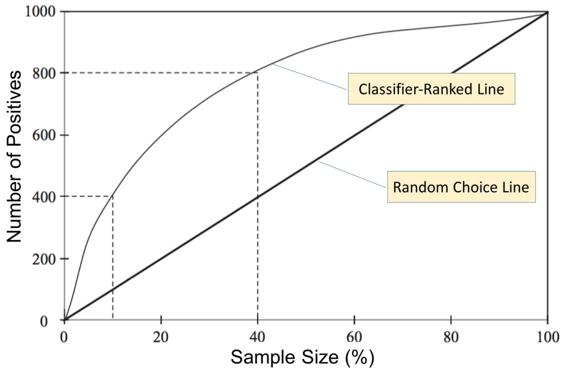
- Probabilities can be converted to a crisp value with different techniques, depending on the number of classes (binary or multiclass)
  - *binary* – set a threshold for the positive class
  - *multiclass* – output the class with the maximum probability

Binary – Lift Chart

- Used to evaluate various scenarios, depending on the application
- Consider a dataset with 1000 positives and apply a probabilistic classification scheme
- Sort all the classified elements for decreasing probability of positive class
- Make a bi-dimensional chart with axes
  $x = \textit{sample size},\ y = \textit{number of positives in sample}$
- Only the rank is important, not the specific probability

Lift Chart

- The straight line plots the number of positives obtained with a random choice of a sample of test data
- The curve plots the number of positives obtained drawing a fraction of test data with decreasing probability
- The larger the area between the two curves, the best the classification model



ROC Curve

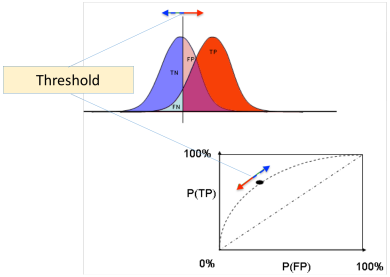
Receiver-Operator Characteristic

History: interpretation of radar signals during WWII

- Tradeoff between hit rate and false alarm in a noisy channel
- The noise can be such that the recognition of the transmission is altered
- The noise alters the two levels according to a gaussian distribution
- Problem: set the positive/negative threshold in order to maximize the tradeoff above, according to application–dependent requirements

ROC Curve

- With less noise the two gaussian curves are better separated
- Moving the threshold towards right increases both the rate of true positives and false positives caught
- The area between the non–discrimination line and the ROC curve is a quality index of the line
- The maximum area is the upper left triangle



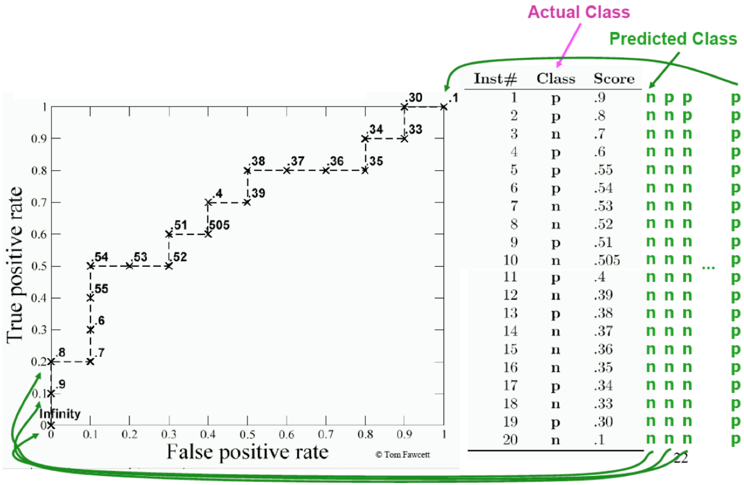
[a]

[a] Image from Wikipedia
TN = blue + cyan = probability of a negative to be caught
FN = cyan = probability of a negative to be missed
FP = pink + purple = probability of a positive to be missed
TP = red + purple = probability of a positive to be caught

ROC for a soft classifier

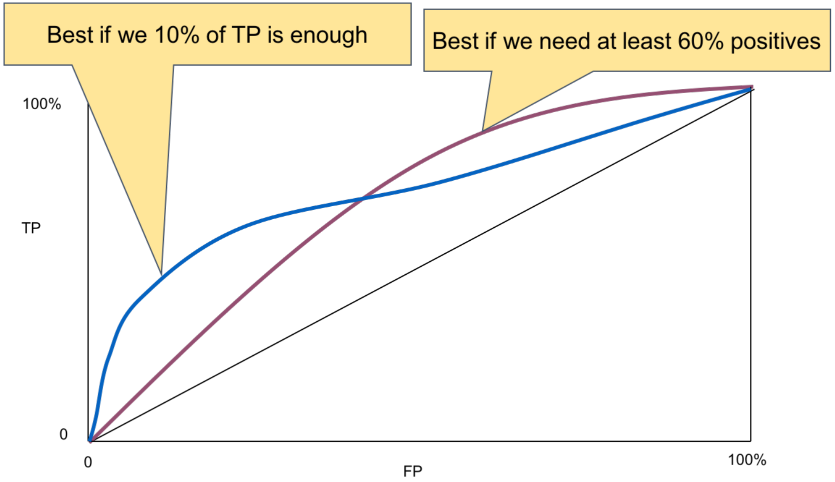
- The soft classifier can be converted into a crisp one by choosing a threshold $\Rightarrow$ predict *positive* if the probability of the test record exceeds the threshold
- Varying the threshold the behavior of the classifier changes, by changing the ratio of TP and FP
- Threshold steps allow to track the ROC curve
    - sort the test elements by decreasing positive probability
    - set the threshold to the highest probability, set TP and FP to zero
    - repeat
        - update the number of TP and FP with probability from the threshold to 1
        - draw a point in the curve
        - move to next top probability of positive
    - end repeat

Drawing the ROC curve for a soft classifier



Inst#	Class	Score				
1	p	.9	n	p	p	p
2	p	.8	n	n	p	p
3	n	.7	n	n	n	p
4	p	.6	n	n	n	p
5	p	.55	n	n	n	p
6	p	.54	n	n	n	p
7	n	.53	n	n	n	p
8	n	.52	n	n	n	p
9	p	.51	n	n	n	p
10	n	.505	n	n	n	p
11	p	.4	n	n	n	p
12	n	.39	n	n	n	p
13	p	.38	n	n	n	p
14	n	.37	n	n	n	p
15	n	.36	n	n	n	p
16	n	.35	n	n	n	p
17	p	.34	n	n	n	p
18	n	.33	n	n	n	p
19	p	.30	n	n	n	p
20	n	.1	n	n	n	p

Drawing the ROC curve for a soft classifier



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  URL http://dx.doi.org/10.1177/001316446002000104.