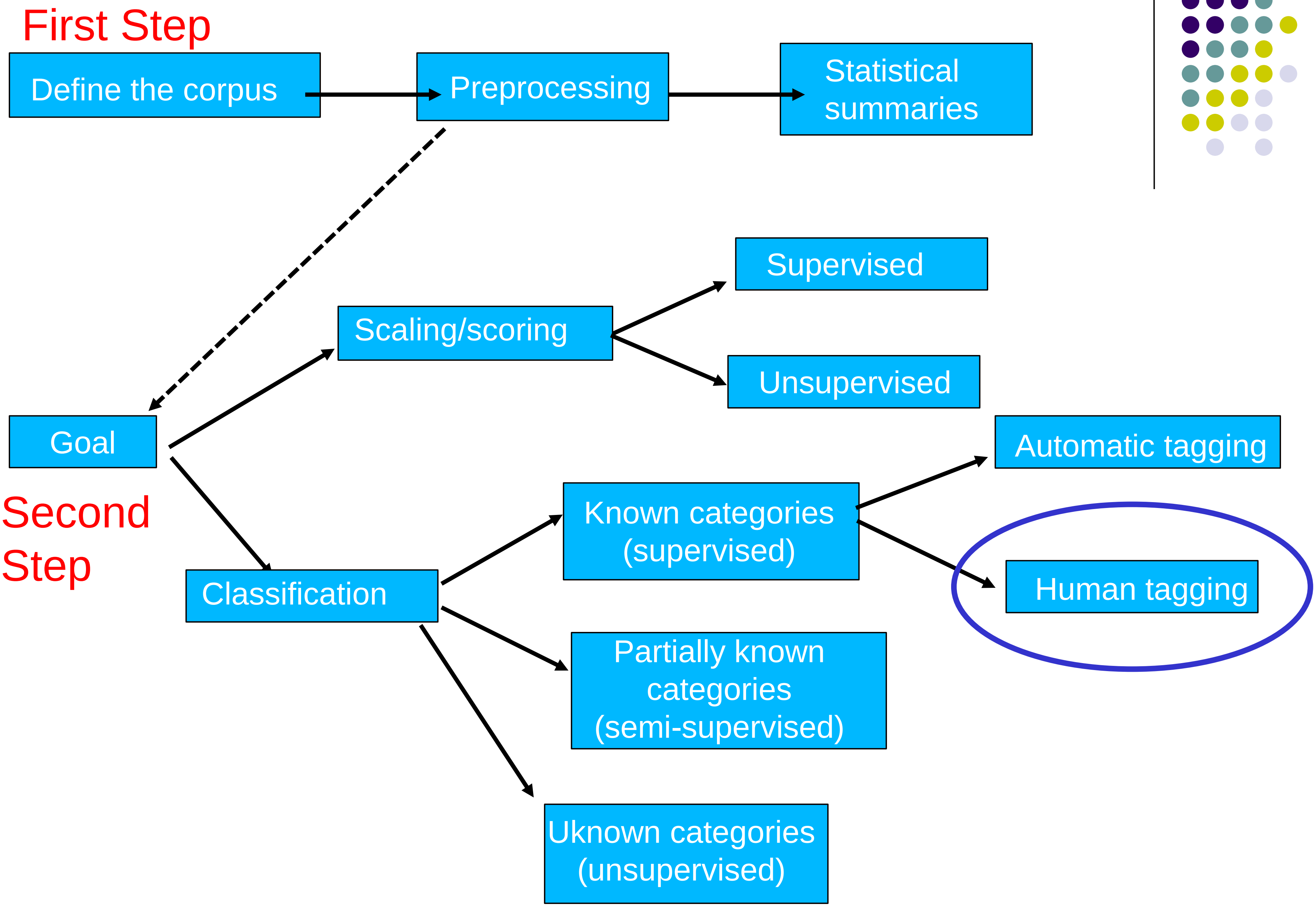
Big Data Analytics

Lecture 4/B
Cross-validation

UNIVERSITÄT LUZERN



First Step

Define the corpus

Preprocessing

Statistical summaries

Goal

Second Step

Scaling/scoring

Supervised

Unsupervised

Classification

Known categories (supervised)

Automatic tagging

Human tagging

Partially known categories (semi-supervised)

Uknown categories (unsupervised)

Reference

✓ Grimmer, Justin, and Stewart, Brandon M. (2013). Text as Data: The Promise and Pitfalls of Automatic Content Analysis Methods for Political Texts. *Political Analysis*, 21(3): 267-297

✓ Curini, Luigi, and Robert Fahey (2020). Sentiment Analysis and Social Media. In Luigi Curini and Robert Franzese (eds.), *SAGE Handbook of Research Methods is Political Science & International Relations*, London, Sage, chapter 29

✓ Cranmer, Skyler J. and Desmarais, Bruce A. (2017) What Can We Learn from Predictive Modeling?, *Political Analysis*, 25: 145-166

Validation

THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

Validation

Since the ultimate goal of supervised learning is to find generalizable patterns of association, models must be **selected based on their ability to generate good out-of-samples predictions (i.e., good predictions on the test-set)**

However, it is impossible to evaluate a model's performance on the universe of unsampled test documents (i.e., you do not know by definition their “true” class-labels of the documents in the test-set after all!), so an approximate measure of performance must be devised

Validation

Supervised methods are designed to automate the hand coding of documents into categories as we have already noticed

If a method is performing well, it will **directly replicate the hand coding**. If it performs poorly, it will fail to replicate the coding – instead introducing serious errors

This clear objective implies a **clear standard for evaluation**: comparing the output of machine coding to the output of hand coding. From here the idea of **validation**!

Validation

The *ideal validation* procedure would divide the data into **three subsets**

1. Initial model fitting would be performed on the training-set
2. Once a final model is chosen, *a second set of hand-coded* documents - the *validation set* - would be used to assess the performance of the model
3. The final model would then be applied to the test to complete the classification

Validation

This approach to validation is difficult to apply in most settings. But **cross-validation** (also called: **K-fold validation**) can be used to replicate this ideal procedure

Validation

In K-fold cross-validation, the training set is randomly partitioned into some groups (say two: K1 and K2)

For each group, the first model is trained on K1, then applied to the K2 to assess performance; similarly a model is trained on the K2 and then applied to K1 to assess performance

Then you take the average across the results you get in the two scenarios

Validation

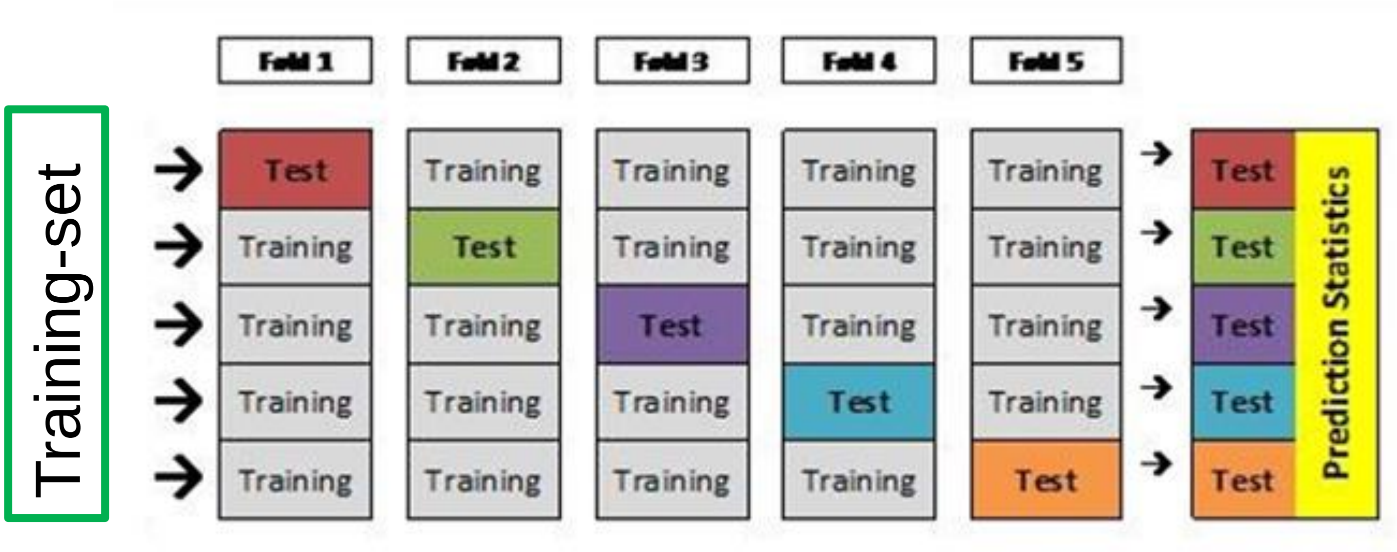
And if you want to run a K-fold cross-validation with K larger than 2?

The algorithm is as follow:

1. Randomly split the data set into k-subsets (or k-fold) (for example 5 subsets)
2. Reserve one subset and train the model on all other subsets (4 in this case)
3. Test the model on the reserved subset and record the prediction error
4. Repeat this process until each of the k subsets has served as the test set
5. Compute the average of the k recorded errors. This is called the **cross-validation error** serving as the performance metric for the model

Validation

So, for example, with K-fold cross-validation=5…



Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	
Test	Training	Training	Training	Training	Test
Training	Test	Training	Training	Training	Test
Training	Training	Test	Training	Training	Test
Training	Training	Training	Test	Training	Test
Training	Training	Training	Training	Test	Test

Validation

How to choose right value of k?

Lower value of k is more biased and hence undesirable. On the other hand, higher value of k is less biased, but can suffer from large variability

In practice, one typically performs k-fold cross-validation using k = 5 or k = 10, as these values have been shown empirically to yield test error rate estimates that suffer neither from excessively high bias nor from very high variance

Validation

REMEMBER: **Cross-validation** is the **only way** to control if the ML algorithm you are using is doing a good job or not (unless you are ready to believe in that by fiat)!

Moreover, cross-validation **avoids overfitting** by focusing on **out-of-sample prediction** and **selects the best model** for the underlying data from a set of candidate models

Validation

Which statistics (or **performance metrics**) should we use to *assess model performance*?

There are several of them, but we are going to focus on three metrics for individual classifiers with text-analysis

Validation

Accuracy: proportion of correctly classified documents

While of course we want this score to be as high as possible, it can also be important to look at the two components which make up that score, known as **recall** and **precision**

Validation

Recall or **Sensitivity** (for a category k) is a measure of what proportion of documents of a given category the algorithm correctly identified; so for example, if there were 10 documents of the category “positive” in the data set, and the algorithm correctly identified 8 of them, we would say that this algorithm has “recall of 0.8 for the category *positive*”

- ✓ given that a human coder labels a document as belonging to category k, what is the chance the machine identifies the document?

Validation

Precision or **Positive Predictive Value** (for a category k) on the other hand is a measure of how many of the times the algorithm identified a category were actually correct, as against how many times were false positives. In the above example, where the algorithm correctly identified 8 of the 10 documents as *positive*, perhaps the algorithm also miss-identified 4 other documents as *positive* - so 8 out of its 12 *positive* classifications were correct, allowing us to say that it has a “precision of 0.667 for the category *positive*”

- ✓ given that the machine guesses category k, what is the probability that the machine made the right guess?

Validation

The aggregate of the recall and precision scores for a category is known as the **f1 score**

More precisely, the traditional F-measure or balanced F-score (**f1**) is the harmonic mean of precision and recall:

f1 = (2 * precision * recall) / (precision + recall)…

…where the highest level of performance (of f1) is equal to 1 and the lowest 0

Validation

The **average of the f1 scores for all the categories** is a reasonable rough measurement of the performance of the algorithm (more than accuracy alone!)

However, before using the algorithm for any serious analysis work, it is always *advisable also to take a look* at the precision and recall scores for individual categories - you may find that a category you are planning to use in your analysis actually has very high rate of false-positive or false-negative identifications, which could cause serious problems for your results

Let’s an example on how to compute the statistics we discussed up to now from the ***Confusion matrix***

Performance metrics

Confusion matrix

	Actual label	
Classification (algorithm)	Black	White
Black	True Black	False Black
White	False White	True White

$$\text{Accuracy} = \frac{\text{TrueBlack} + \text{TrueWhite}}{\text{TrueBlack} + \text{TrueWhite} + \text{FalseBlack} + \text{FalseWhite}}$$

$$\text{Precision}_{\text{Black}} = \frac{\text{TrueB}}{\text{TrueB} + \text{FalseB}}$$

→ Think horizontally

$$\text{Recall}_{\text{Black}} = \frac{\text{TrueB}}{\text{TrueB} + \text{FalseW}}$$

→ Think vertically

$$f_{1\text{Black}} = \frac{2 * \text{precisionB} * \text{recallB}}{\text{precisionB} + \text{recallB}}$$

Performance metrics: an example

	Actual label	
Classification (algorithm)	Black	White
Black	800	100
White	50	50

$$\text{Accuracy} = \frac{800 + 50}{800 + 50 + 100 + 50} = 0.85$$

$$\text{Precision}_{\text{Black}} = \frac{800}{800 + 100} = 0.88$$

$$\text{Recall}_{\text{Black}} = \frac{800}{800 + 50} = 0.94$$

$$f_{1\ \text{Black}} = \frac{2*.88*.94}{.88 + .94} = 0.91$$

Performance metrics

Confusion matrix

	Actual label	
Classification (algorithm)	Black	White
Black	True Black	False Black
White	False White	True White

$$\text{Accuracy} = \frac{\text{TrueBlack} + \text{TrueWhite}}{\text{TrueBlack} + \text{TrueWhite} + \text{FalseBlack} + \text{FalseWhite}}$$

$$\text{Precision}_{\text{White}} = \frac{\text{TrueW}}{\text{TrueW} + \text{FalseW}} \longrightarrow$$

Think horizontally

$$\text{Recall}_{\text{White}} = \frac{\text{TrueW}}{\text{TrueW} + \text{FalseB}} \longrightarrow$$

Think vertically

$$f_{1\text{White}} = \frac{2 * \text{precisionW} * \text{recallW}}{\text{precisionW} + \text{recallW}}$$

Performance metrics: an example

	Actual label	
Classification (algorithm)	Black	White
Black	800	100
White	50	50

$$\text{Accuracy} = \frac{800 + 50}{800 + 50 + 100 + 50} = 0.85$$

$$\text{Precision}_{\text{White}} = \frac{50}{50 + 50} = 0.5$$

$$\text{Recall}_{\text{White}} = \frac{50}{50 + 100} = 0.33$$

$$f_{1\ \text{White}} = \frac{2 * .5 * .33}{.5 + .33} = 0.39$$

Performance metrics

In this example you are going to have a single Accuracy value=0.85

Then you could take the **average of the F1 scores** for the classes as another (and more reliable) measure of the performance of the algorithm

In our case: (.91+.39)/2=.65

You see the difference here between Accuracy and the averaged F1 score!

This difference is due that we are doing well with the Black class, but relative poorly with the White class

Rule-of-thumb: everytime you notice a market difference between Accuracy and F1 score, there are problems for your model!!!

Validation

For example, if there were 96 cats and only 4 dogs in the training-set (i.e., a very **imbalanced** training-set: we will be back on this point later on!), a particular classifier **might classify all the observations (but one) as cats**

The overall accuracy would be then…how much?

Performance metrics: an example

	Actual label	
Classification (algorithm)	Cats	Dogs
Cats	95	4
Dogs	1	0

$$\text{Accuracy} = \frac{95 + 0}{95 + 4 + 1 + 0} = 0.95$$

Accuray seems high, but compared to a natural benchmark (i.e., *a dull algorithm that simply assigns all the observations to the most frequent class*)?

In this case: random draw=96% of Accuracy!

Validation

Moreover, in this same circumstance, the classifier would have a **recall rate (sensitivity)** for the *dog class* equals to…? And for the cats equals to…? [think vertically!]

Performance metrics: an example

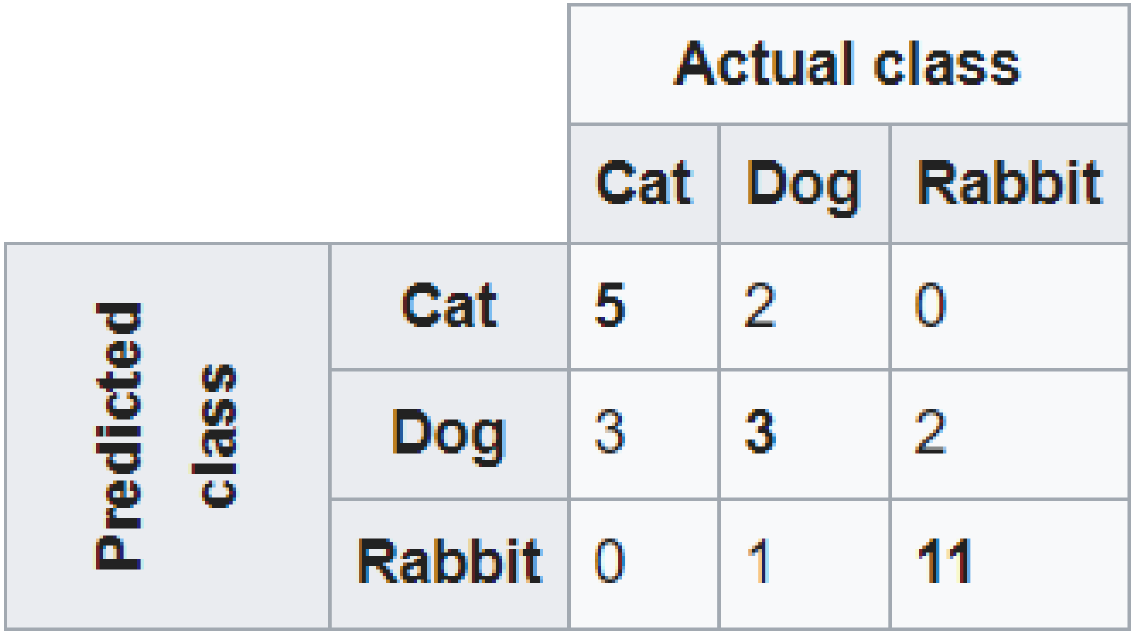
	Actual label	
Classification (algorithm)	Cats	Dogs
Cats	95	4
Dogs	1	0

$$\text{Accuracy} = \frac{95+0}{95+4+1+0} = 0.95$$

$$\text{Recall}_{\text{Dogs}} = \frac{0}{0+4} = 0$$

$$\text{Recall}_{\text{Cats}} = \frac{95}{95+1} = 0.989$$

Validation: another example with 3 categories

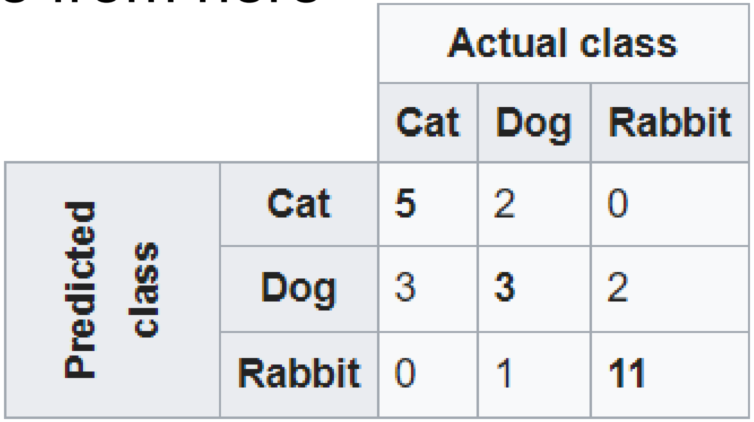


		Actual class		
		Cat	Dog	Rabbit
Predicted class	Cat	5	2	0
	Dog	3	3	2
	Rabbit	0	1	11

Here **Accuracy** is equal to the ratio between the sum of the diagonal (i.e., the sum of «True Positive») and the total number of observations, i.e., (5+3+11)/(5+2+3+3+2+1+11)=0.704

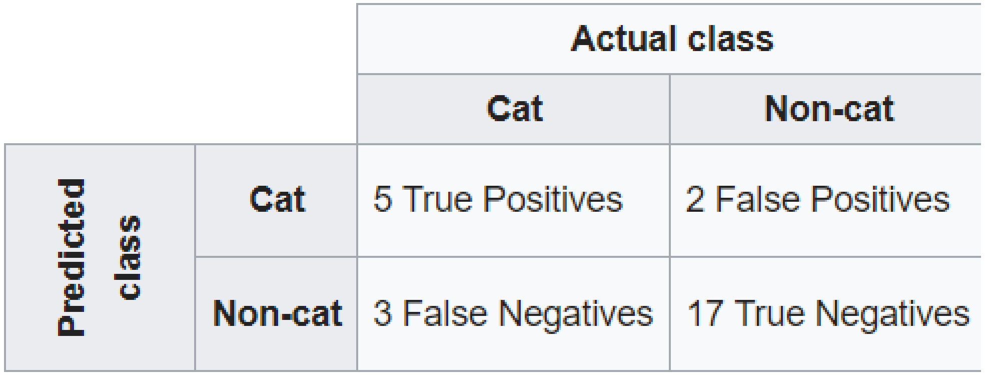
Validation

For each category *k* we can move from here



		Actual class		
		Cat	Dog	Rabbit
Predicted class	Cat	**5**	2	0
	Dog	3	**3**	2
	Rabbit	0	1	**11**

to here (example for the “cat” category)



		Actual class	
		Cat	Non-cat
Predicted class	Cat	5 True Positives	2 False Positives
	Non-cat	3 False Negatives	17 True Negatives

Validation

Then:

In the case, Precision for the cat class is: 5/(5+2)=0.71

Recall for the cat class is: 5/(5+3)=0.625

f1 for the cat class is: 2*(0.625*071)/(0.625+071)=0.66

You can do the same thing for the dog and the rabbit cases, and then averaging across values to have a sense of the overall performance of your model

Validation

Depending on the application, scholars may conclude that the supervised method is able to sufficiently replicate human coders. A largely employed rule-of-thumb is getting accuracy>.85 for example (or f1>.75) (at least when you are dealing with *just 2 categories*)

Or, additional steps can be taken to improve accuracy, including trying to apply other ML algorithms or…

Validation

…Most algorithms also have a range of “**hyper-parameters**” (or “tuning parameters”) – assumptions and modifiers which are used to fine-tune the model and which can be set to different values prior to training – that can significantly impact performance (remember about the number of trees in RF)

Finding the right set of hyper-parameters for a certain task and a specific data set is also largely a case of trial and error, and it can only be done once again via cross-validation!

Validation

Some packages in R (such as `Caret` or `h2o` or the same `Quanteda` with the library `quanteda.classifiers`) provide ways to automate this task; this is known as a "grid search", allowing researchers to exhaustively search through every combination of a set of hyper-parameters to find the best performing model

This process can take a lot of time – often in the order of several hours for algorithms with complex sets of parameters – but often yields better performance than the default parameter set

Validation

Summing up: the purpose of cross-validation is **model checking**!

Accordingly, cross-validation allows you to:

- ✓ **select among different machine-learning algorithms**...(remember the **No Free Lunch Theorem!** No machine learning algorithm is always better at predicting new, unobserved, data points universally)
- ✓ ..and to identify the **better hyperparameters setting for a given ML algorithm**

As a result always run a cross-validation before classifying the test-set to select the best ML algorithm given your corpus!

Validation: a summary

Two possible routes in this regard according to how you want to deal with the **hyper-parameters**:

First route (to success…)

a) You keep the default hyper-parameters of your ML algorithms;

b) you run a CV on each of such ML algorithms

c) you select the one (or two) with the best performance on CV

d) you fine-tune the hyper-parameters on such model(s)

e) you re-run CV just on them

f) you keep the ML algorithm that performs better in the CV

Validation: a summary

Two possible routes in this regard according to how you want to deal with the **hyper-parameters**:

Second route (to success…)

a) You fine-tune the hyper-parameters on each of the your ML algorithms you want to test

b) you run CV on each of them

c) you keep the ML algorithm that performs better in the CV