

# Data Analysis and Model Classification

## Guidesheet I-3: Model selection and nested cross-validation

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This guidesheet should help you understand better how to select the best features for your classifier and crucially, how to correctly estimate the performance of a model (classifier) on an unseen and independent dataset (**features**). In the previous guidesheet, we put into practice the theory behind LDA/QDA classifiers, and also had a brief introduction to model selection. We saw that a model has a certain number of parameters that are automatically optimized using the training set. However, you might have noticed that we had an additional parameter which was not automatically tuned: the choice of the classifier type (*diaglinear*, *diagquadratic*, *linear* or *quadratic*). We call it a **hyperparameter**, and the way it is chosen is called *hyperparameter optimisation* or *model selection*. Other hyperparameters are for example the specific features and the total number of features used. We will do the feature selection by ranking features according to a metric and keeping only the **first  $N_{sel}$  best features**.

### Cross-validation for hyperparameter optimization

We will use cross-validation for model selection. This means that each classifier trained with a different  $N_{sel}$  will be considered as a different *model* and our goal is to select the best one. For this, we will analyse how the **class-averaged classification error** evolves with  $N_{sel}$ . To rank the features, use the **rankfeat()** function with the *Fisher* method (you need to download the function from moodle). This function takes **features and labels as inputs**, and outputs a list of feature ordered **by discriminative power**.<sup>1</sup> In each fold, test your classifier **with the single best feature**, save the training and test error. Repeat these steps with the **two best features**, save the training and test error, and **so on**. With every feature that you add, you change the model you are testing. This means that you will end up with a matrix of test errors of **size  $N \times K$** , where  $N$  is the number of models you tried out and  $K$  is the number of folds. The decision about which **number of features** is good for your model will be based on the **average of all folds**.

Remember the golden rule: the cross-validation test samples must be independent from the training set and not taken into account for model fitting. You must use **only** the training folds (9/10 of the folds for 10-fold cross-validation). Otherwise, you will **overfit**!<sup>2</sup>

#### Design questions






- How would you implement your cross-validation? Write the implementation on a sheet of paper in pseudo-code.
- What is the role of your **train set and test set**?
- Where will you put the **feature selection**? *Inside* or *outside* the cross-validation loop. 

#### Hands on

- Implement the cross-validation with *Fisher*-based feature selection and save both training and test error for each fold and each number of features. Use a **diaglinear** classifier.

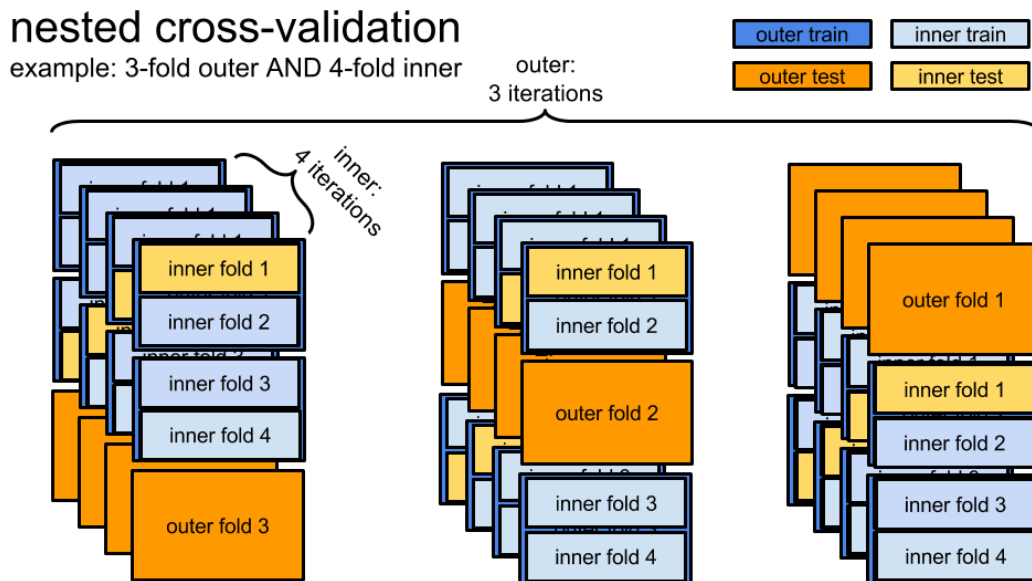
<sup>1</sup>That means that if the first three values are 23,32,1, the most discriminative feature is feature #23, followed by feature #32 and feature #1

<sup>2</sup><https://www.youtube.com/watch?v=DQWI1kvmwRg> or alternatively <https://en.wikipedia.org/wiki/Overfitting>

- Plot training and test error for every number of features. You can use `plot(err, 'b')`; to plot the error for every cross-validation fold (for 'b', rows = number of features, columns = folds) and then `hold on; plot(mean(err,2), 'b', 'LineWidth', 2)`; to plot the mean error across folds. Do the same for the test error with another color.
- Do the two curves behave differently? 
- Based on these curves, what is the optimal number of features? 
- We picked the final model with the best performance. This is a cherry-picking process which means risky because we simply picked the best one **with only one-time comparison without any theoretical support**. To illustrate the problem in an easy way, you can implement a 4-fold cross-validation for a random classifier.<sup>3</sup> The **theoretical error is 50%**. How different the mean error across folds is from it? Repeat **1,000**  **times the cross-validation** and save the mean test error for each repetition.  Among these 1,000 values, what is the minimum test error? what do you conclude? 

## Nested cross-validation for performance estimation

The error obtained with **simple** cross-validation is a **biased** estimation of the true error. This means, that although our **simple** cross-validation loop allows us to choose the best hyperparameters of our model (e.g. number of features), we are unsure about the true performance of our model, and we would need a new unseen dataset to test and to accurately estimate the test error. To do this optimally on a small dataset, we will do an *outer* cross-validation to test the performance of the classifier while the model selection will be performed in an *inner* cross-validation inside of each fold of the *outer* cross-validation.



**Figure 1:** Graphical representation of nested cross-validation: three outer folds and four inner folds. Note that you need to have labels for all the data that you are using for cross-validation.

From now on, we will call the error computed on a test fold of the outer cross-validation *test* error, while the “test” error computed for each hyperparameter value during the *inner* cross-validation will be called the *validation* error. The *validation* error, which helps us assess the hyperparameters, can be computed as many times as we want (once per model and inner fold). Therefore it will be saved in a  $N \times K_{in}$  matrix. Where  $N$  is the number of models that you try and  $K_{in}$  is the number of inner folds. The *test* error can be computed only once per outer fold, to assess the final performance of the model. Therefore it will be saved in a  $1 \times K_{out}$  vector, where  $K_{out}$  is the number of outer loop folds.

<sup>3</sup>A random classifier is very stupid: to classify a sample, it simply flips a coin to decide on whether the output will be 0 or 1.

## Design questions

- How would you implement your inner and outer cross validation loops ? Write the implementation on a sheet of paper in pseudo-code.
- What is the role of your inner train set, inner test set, outer train set, outer test set?
- Where will you put the feature selection? Inside the inner cross-validation? Inside the outer cross-validation? Outside the outer cross-validation? Or any combination of the preceding?

## Hands on



- Implement the nested cross-validation with *Fisher*-based feature selection. In each *outer* cross-validation fold, select the best model. The best model is the one that has the lowest mean validation error across inner cross-validation folds. Save the optimal hyperparameter ( $N_{sel}$ ) and the corresponding minimum validation error (*optimal validation* error) and associated training error (*optimal training* error). Use a *diaglinear* classifier



- How does the *hyperparameter* differ across folds? Compare the median error of the *hyperparameters* to the *hyperparameter* found in the simple cross-validation of the last section?



- Make a **boxplot** of the distribution of *optimal training, optimal validation* and *test* error. How do they differ and why?



- Do the same but vary the classifier type as a *hyperparameter on top of the number of features*. How does the classifier type change from one fold to another?



- Does your *final model* change?

- Test on Kaggle your final model.