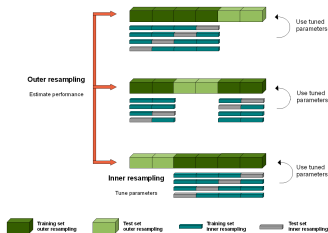


# Introduction to Machine Learning

## Nested Resampling



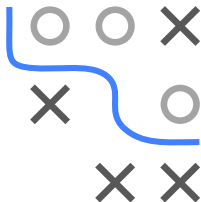
### Learning goals

- Understand how the 3-way split of the data can be generalized to nested resampling
- Understand the goal of nested resampling
- Be able to explain how resampling allows to estimate the generalization error

# NESTED RESAMPLING

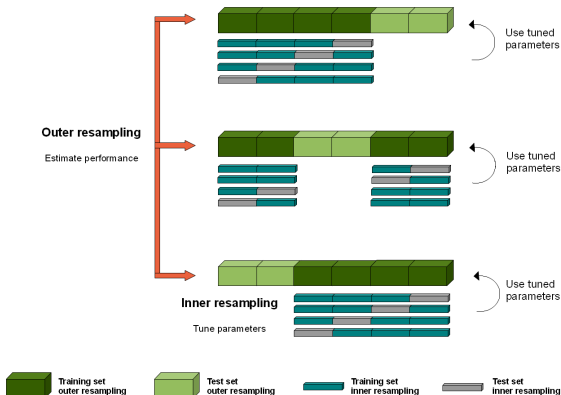
Just like we can generalize hold-out splitting to resampling to get more reliable estimates of the predictive performance, we can generalize the training/validation/test approach to **nested resampling**.

This results in two nested resampling loops, i.e., resampling strategies for both tuning and outer evaluation.



# NESTED RESAMPLING / 2

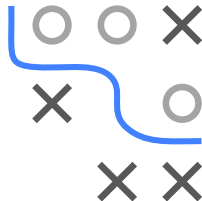
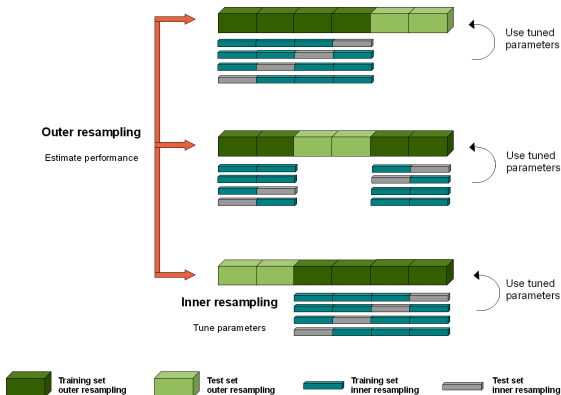
Assume we want to tune over a set of candidate HP configurations  $\lambda_i; i = 1, \dots$  with 4-fold CV in the inner resampling and 3-fold CV in the outer loop. The outer loop is visualized as the light green and dark green parts.



# NESTED RESAMPLING / 3

In each iteration of the outer loop we:

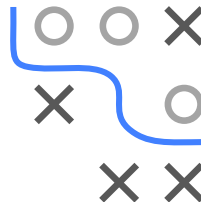
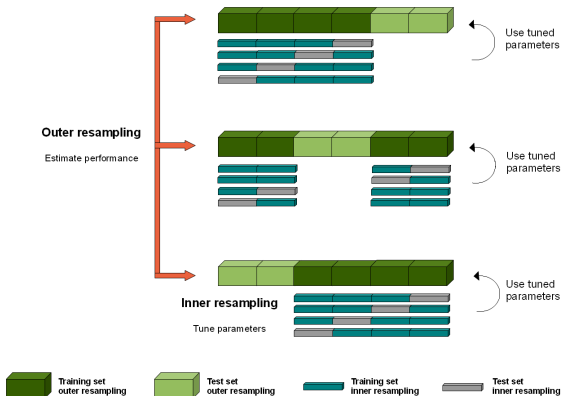
- Split off the light green testing data
- Run the tuner on the dark green part of the data, e.g., evaluate each  $\lambda_i$  through fourfold CV on the dark green part



# NESTED RESAMPLING / 4

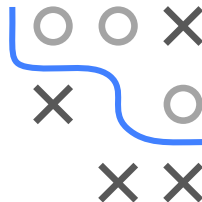
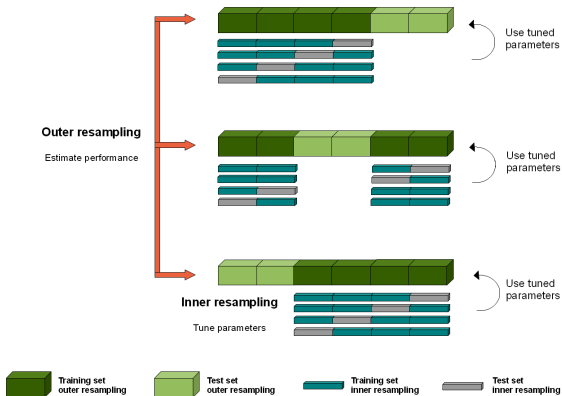
In each iteration of the outer loop we:

- Return the winning  $\lambda^*$  that performed best on the grey inner test sets
- Re-train the model on the full outer dark green train set
- Evaluate it on the outer light green test set



# NESTED RESAMPLING / 5

The error estimates on the outer samples (light green) are unbiased because this data was strictly excluded from the model-building process of the model that was tested on.



# NESTED RESAMPLING - INSTRUCTIVE EXAMPLE

Taking again a look at the motivating example and adding a nested resampling outer loop, we get the expected behavior:

