Introduction to Machine Learning

Tuning: Nested Resampling

compstat-lmu.github.io/lecture_i2ml

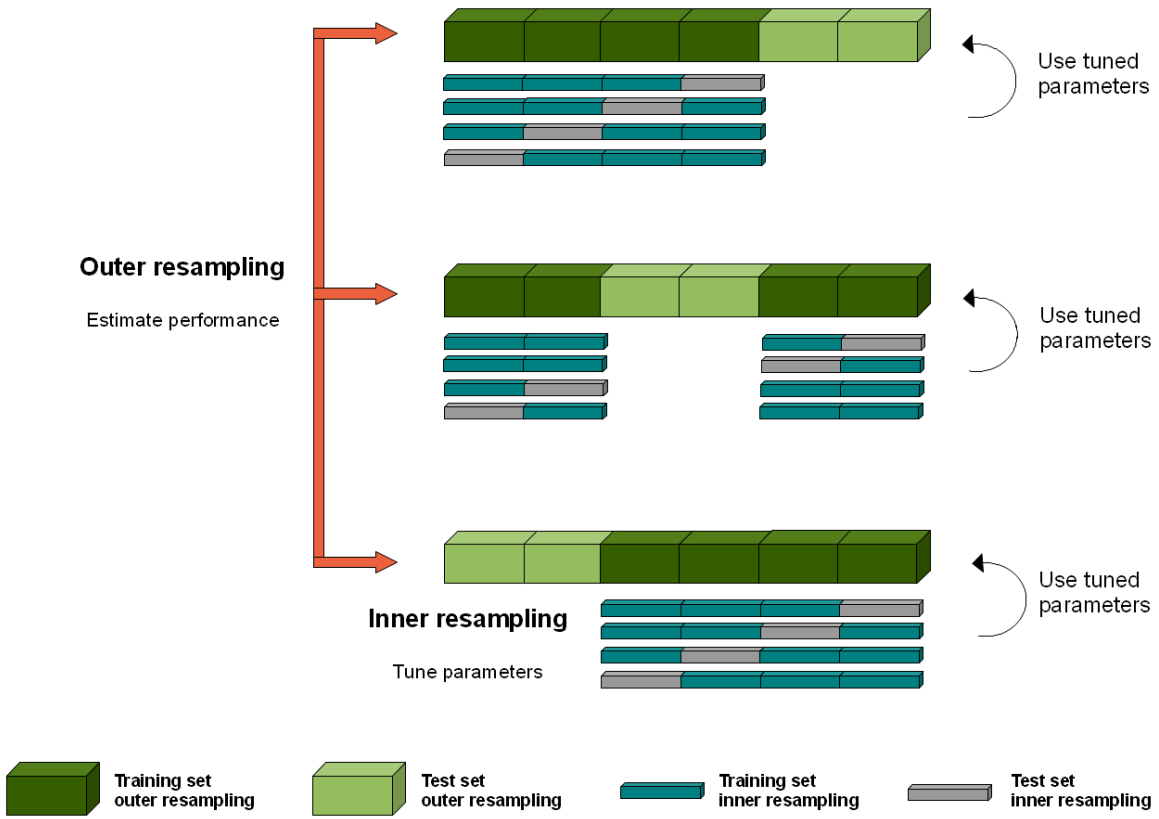
NESTED RESAMPLING

Just like we can generalize holdout 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

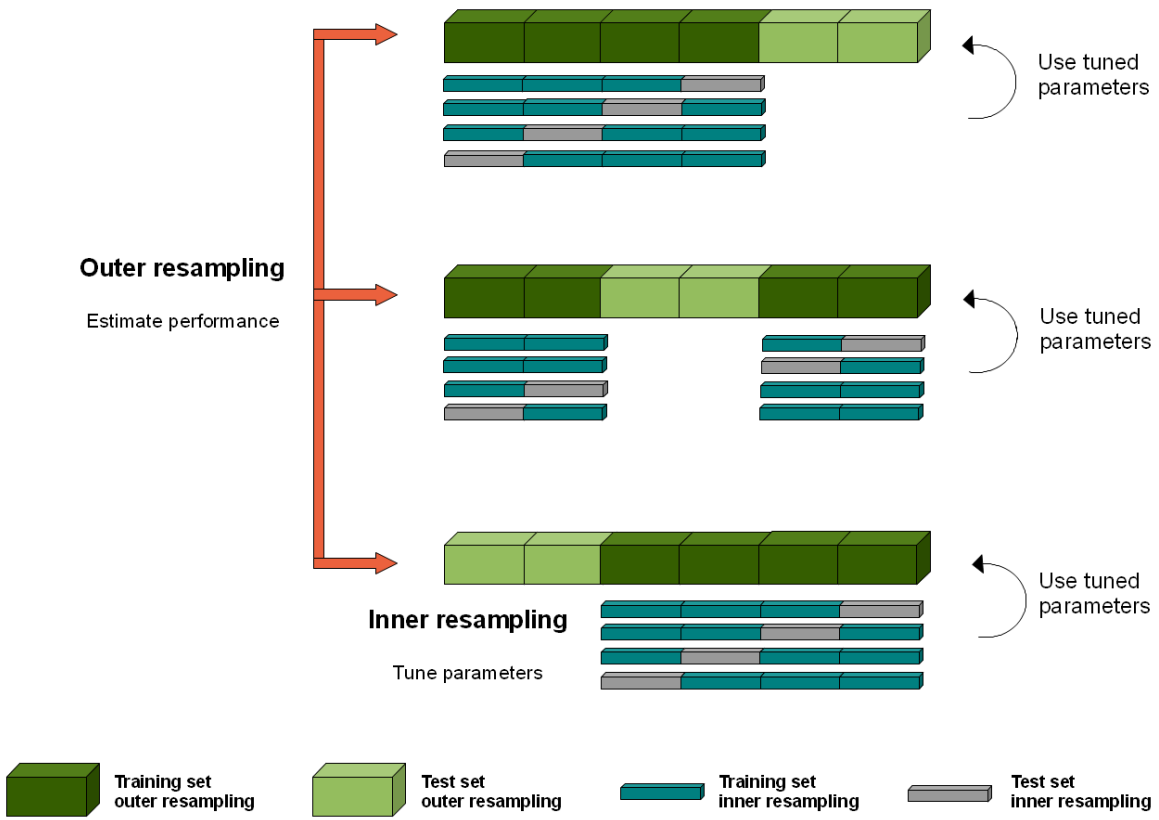
Assume we want to tune over a set of candidate HP configurations $\lambda_i; i = 1, \ldots$ with 4-fold CV in the inner resampling and 3-fold CV in the outer loop. The outer loop is visualized as the light green and dark green parts.



NESTED RESAMPLING

In each iteration of the outer loop we:

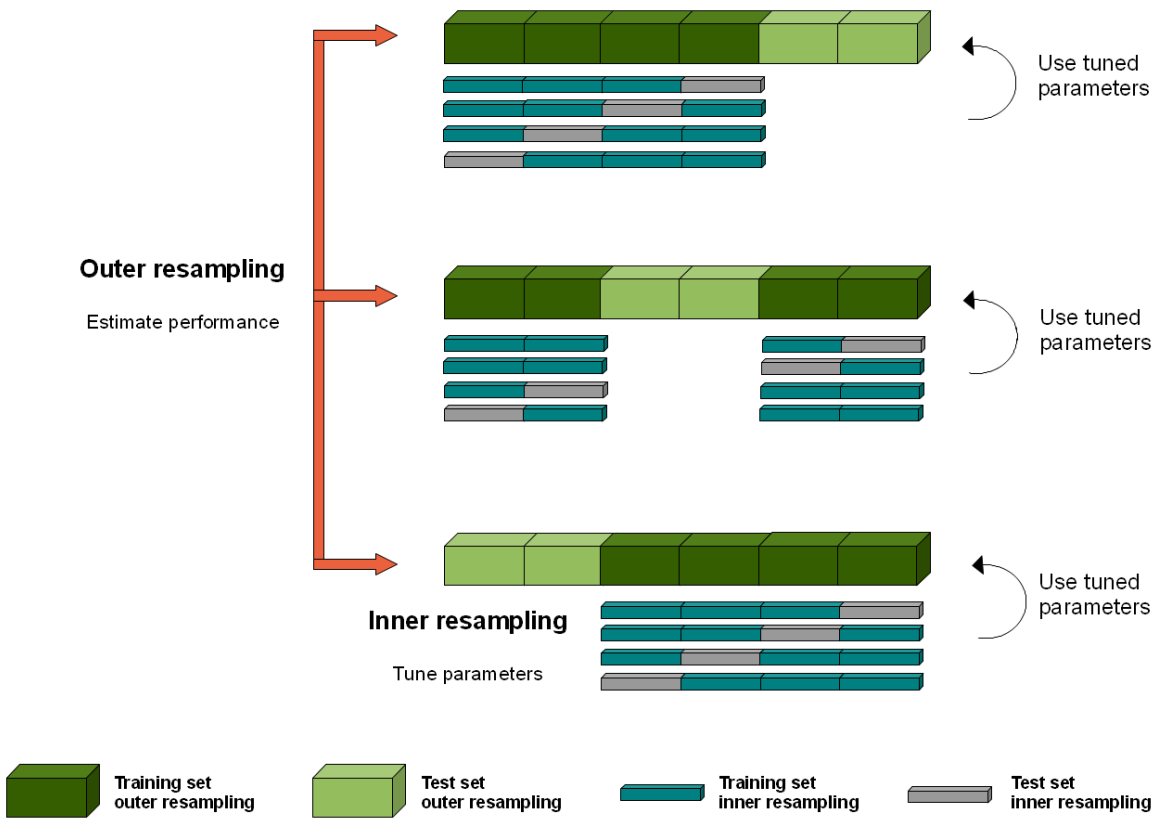
- Split off the light green testing data
- Run the tuner on the dark green part of the data, e.g., evaluate each λ_i through fourfold CV on the dark green part



NESTED RESAMPLING

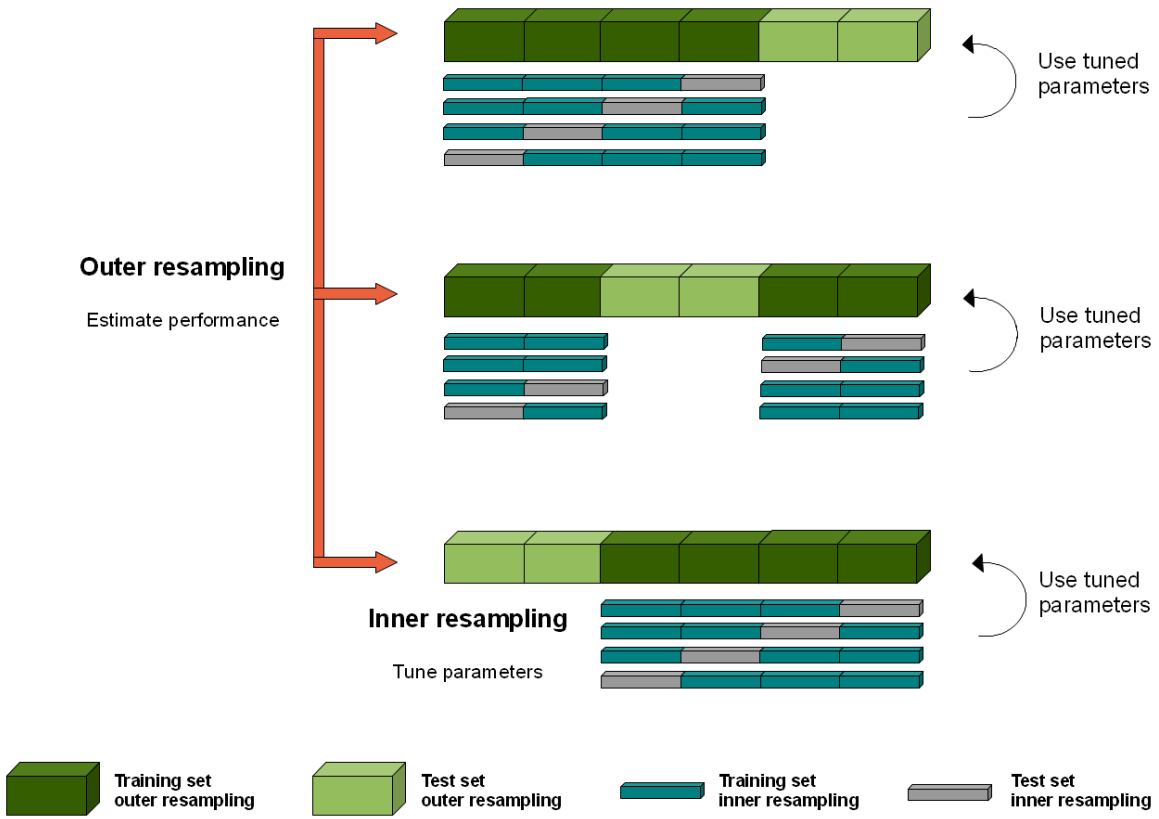
In each iteration of the outer loop we:

- Return the winning λ^* 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

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: