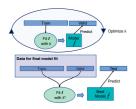
Introduction to Machine Learning

Nested Resampling **Training - Validation - Test**





Learning goals

- Understand how to fulfill the untouched test set principle by a 3-way split of the data
- Understand how thereby the tuning step can be seen as part of a more complex training procedure

TUNING PROBLEM

Remember:

× 0 × × ×

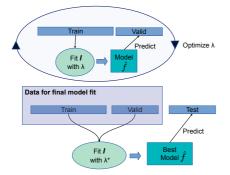
We need to

- select an optimal learner
- without compromising the accuracy of the performance estimate for that learner
- for that we need an untouched test set!

TRAIN - VALIDATION - TEST

Simplest method to achieve this: a 3-way split

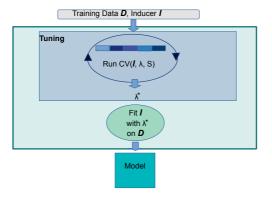
- During tuning, a learner is trained on the training set, evaluated on the validation set
- After the best model configuration λ^* has been selected, we re-train on the joint (training+validation) set and evaluate the model's performance on the **test set**.





TUNING AS PART OF MODEL BUILDING

- Effectively, the tuning step is now simply part of a more complex training procedure.
- We could see this as removing the hyperparameters from the inputs of the algorithm and making it "self-tuning".





TUNING AS PART OF MODEL BUILDING

More precisely: the combined training & validation set is actually the training set for the "self-tuning" endowed algorithm.

