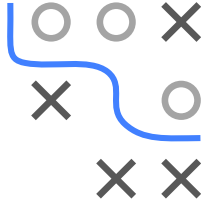
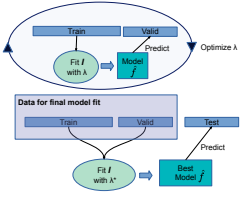
Introduction to Machine Learning



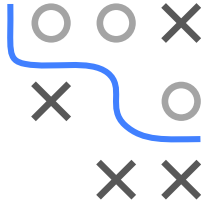
Nested Resampling
Training - Validation - Test



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:

We need to

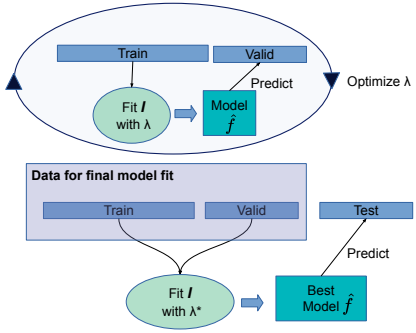
- **select an optimal learner**
- without compromising the **accuracy of the performance estimate** for that learner

– for that we need an **untouched test set**!

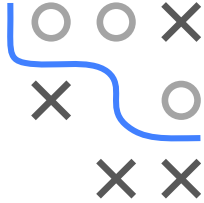
TRAIN - VALIDATION - TEST

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 $\boldsymbol{\lambda}^*$ 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”.