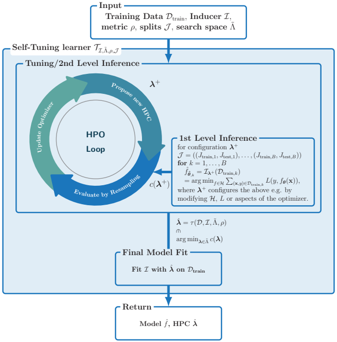
Introduction to Machine Learning

Hyperparameter Tuning - Practical Aspects

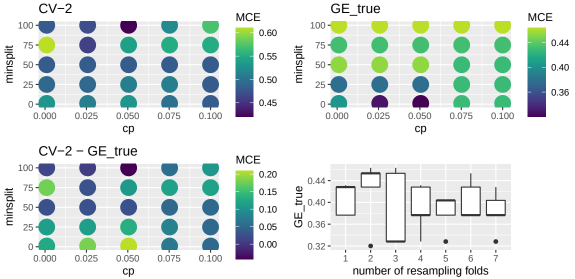


Learning goals

- Understand the possible design choices for HPO
- Know termination criteria of HPO

PRACTICAL ASPECTS OF HPO

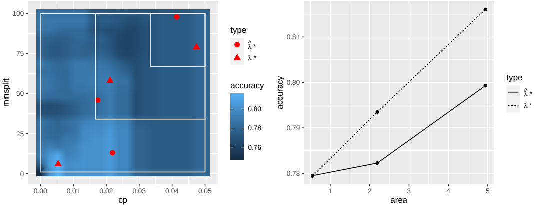
- Choosing resampling
  - Nr of observations, i.i.d assumption for data sampling process
  - Higher resampling rates likely result in a better model; however they are computiationally more expensive



Tuning a CART on the `spirals` data with a k-fold CV (k=1 means here a $2/3$ holdout split) using grid search and estimating the true GE with a very large test set (5 repetitions)

PRACTICAL ASPECTS OF HPO

- Choosing performance measure
  - Desired implications when applying the model in practice
- Choosing a pipeline and search space
  - Numeric HPs of arbitrary size should be tuned on log scale
  - Size of search space results in different trade-offs:
    too small may miss out well performing HPCs;
    too large makes optimization more difficult



Tuning cp and minsplit for a CART on the `titanic` data over 3 increasing rectangular search spaces with random search (candidates number fixed) and comparing the result with the optimal model (found with exhaustive grid search)

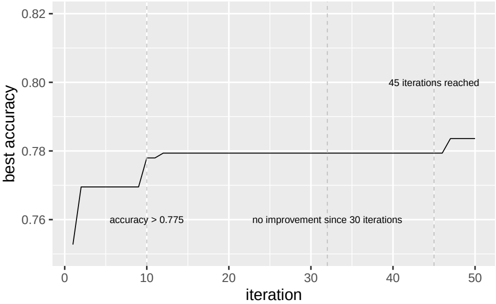
PRACTICAL ASPECTS OF HPO

- Choosing HPO algorithm
  - For few HPS (1-3), grid search can be used
  - BO with GPs for upto 10 numeric HPs
  - BO with RFs handle mixed HP spaces
  - Random search and Hyperband work well as long as the "effective" dimension is low
  - EAs are somewhat in-between BO and RS, can handle very complex spaces, but less sample efficient than BO
  - **Also: use something that's stable and robust! More an aspect of the implementation than the algo!**

PRACTICAL ASPECTS OF HPO

When to terminate HPO

- Specify a certain amount of runtime/budget beforehand
- Set a lower bound regarding $\widehat{\mathrm{GE}}$
- Terminate if performance improvement stagnates



Different stopping points while tunining CART on the `titanic` data depending on which termination criterion is used

PRACTICAL ASPECTS OF HPO

- Warm starts
  - Evaluations (e.g., weight sharing of neural networks)
  - Optimization (intializing with HPCs that worked well before)
- Control of execution
  - Parallelizability of HPO algorithms differs strongly
  - HPO execution can be parallelized at different levels (outer resampling, iteration, evaluation, inner resampling, model fit)