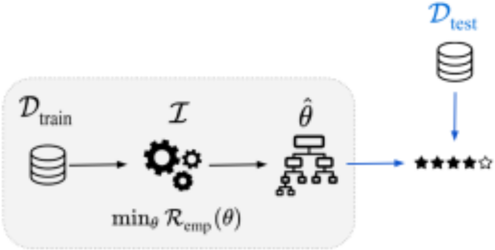
MOTIVATING EXAMPLE / 2

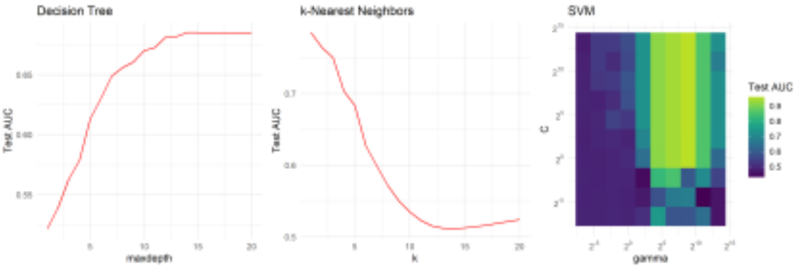
- We are **actually** interested in the **generalization performance** $\mathrm{GE}\left(\hat{f}\right)$ of the estimated model on new, previously unseen data.
- We estimate the generalization performance by evaluating the model $\hat{f} = \mathcal{I}(\mathcal{D}_{\text{train}}, \boldsymbol{\lambda})$ on a test set $\mathcal{D}_{\text{test}}$:

$$\widehat{\mathrm{GE}}_{\mathcal{D}_{\text{train}},\mathcal{D}_{\text{test}}}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho) = \rho\left(\mathbf{y}_{\mathcal{D}_{\text{test}}}, \boldsymbol{F}_{\mathcal{D}_{\text{test}},\hat{f}}\right)$$



MOTIVATING EXAMPLE / 3

- But many ML algorithms are sensitive w.r.t. a good setting of their hyperparameters, and generalization performance might be bad if we have chosen a suboptimal configuration.
- Consider a simulation example of 3 ML algorithms below, where we use the dataset *mlbench.spiral* and 10,000 testing points. As can be seen, variating hyperparameters can lead to big difference in model's generalization performance.



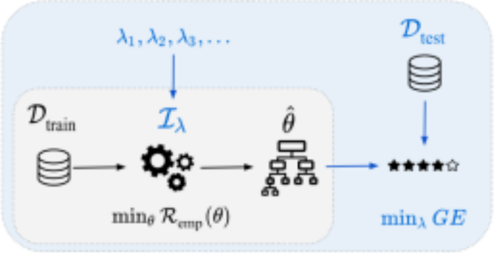
MOTIVATING EXAMPLE / 4

For our example this could mean:

- Data too complex to be modeled by a tree of depth 4
- Data much simpler than we thought, a tree of depth 4 overfits

$\Longrightarrow$ Algorithmically try out different values for the tree depth. For each maximum depth λ, we have to train the model **to completion** and evaluate its performance on the test set.

- We choose the tree depth λ that is **optimal** w.r.t. the generalization error of the model.



MODEL PARAMETERS VS. HYPERPARAMETERS / 2

In contrast, **hyperparameters** (HPs) λ are not optimized during training. They must be specified in advance, are an **input** of the training. Hyperparameters often control the complexity of a model, i.e., how flexible the model is. They can in principle influence any structural property of a model or computational part of the training process.

The process of finding the best hyperparameters is called **tuning**.

Examples:

- Maximum depth of a tree
- k and which distance measure to use for k-NN
- Number and maximal order of interactions to be included in a linear regression model
- Number of optimization steps if the empirical risk minimization is done via gradient descent