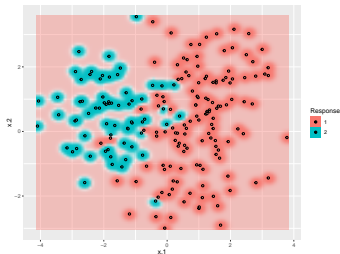


Introduction to Machine Learning

Evaluation: Overfitting

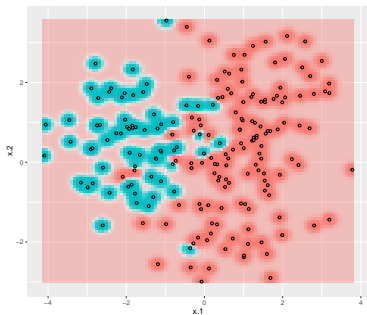


Learning goals

- Understand what overfitting is and why it is a problem
- Learn about countermeasures to overfitting

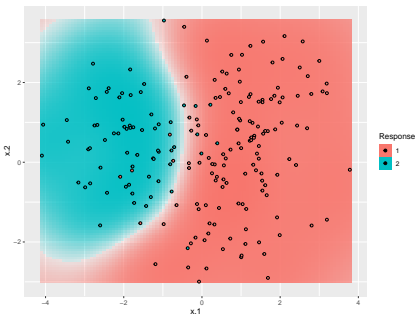
OVERFITTING

Overfitting learner



Better training set performance
(seen examples)

Non-overfitting learner



Better test set performance
(unseen examples)

OVERFITTING

BB: def overfitting We can quantify overfitting as difference between the generalization error and the apparent training error, i.e.

$$\text{GE}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho) - \rho(\mathbf{y}_{\text{train}}, F_{\text{train}}).$$

We can estimate this quantity via e.g. a holdout-split

$$\widehat{\text{GE}}_{\mathcal{D}_{\text{train}}, \mathcal{D}_{\text{test}}}(\mathcal{I}, \boldsymbol{\lambda}, n_{\text{train}}, \rho) - \rho(\mathbf{y}_{\text{train}}, F_{\text{train}}).$$

OVERFITTING

- **Overfitting** is a well-known problem with powerful (non-linear) learning algorithms.
- It occurs when the learner starts modeling patterns in the data that are not actually there, i.e., noise or artifacts in the training data.
→ Too many hypotheses and not enough data to tell them apart.
- Symptoms of overfitting are small training errors that come at the expense of high test errors.
- Recall that our primary focus is on the learner's ability to generalize well to new observations, not fit the training data perfectly.
- In larger data sets overfitting is less of an issue as more data allow for more poor hypotheses to be eliminated, but if the hypothesis space is not constrained, there may never be enough data.

AVOIDING OVERFITTING

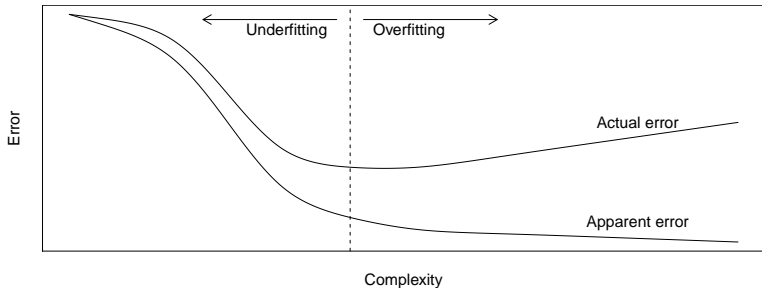
Remedies against overfitting include:

- Use less complex models – e.g., lower-degree polynomials.
- Get more, or better, data – not always possible, but there are techniques to augment existing data, e.g., for image data.
- Apply regularization – many learners come with hyperparameters that enable to constrain complexity.
- Some learners are also eligible for "early stopping", where the learning process is terminated before perfectly fitting (i.e., overfitting) the training data.

In the end, we will always need to balance a trade-off between model fit and generalization ability.

TRADE-OFF BETWEEN COMPLEXITY AND GENERALIZATION ERROR

Apparent error (at training time) and **actual error** (at prediction time) evolve in opposite directions with increasing complexity:



→ We would like to find the optimal level of complexity:
Hit the sweet spot for the given amount of data where generalization error becomes minimal.