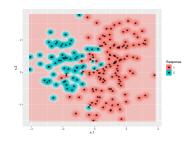
# **Introduction to Machine Learning**

# **Evaluation: Overfitting and Underfitting**





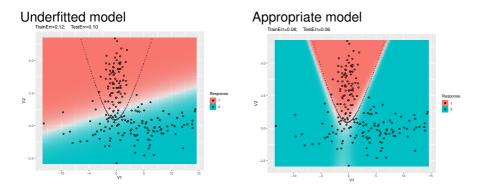
#### Learning goals

 Understand definitions of overfitting and underfitting

### **UNDERFITTING**

- Occurs if model does not reflect true shape of underlying function
- Hence, predictions will be less good as they could be
- High train error and high test error
- Hard to detect, as we don't know what the Bayes error is for a task

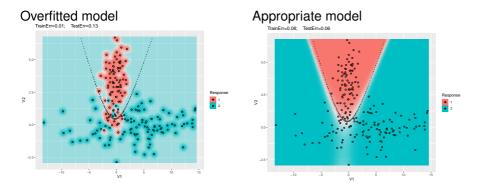




#### **OVERFITTING**

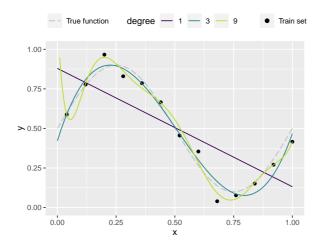
- Overfitting occurs when the model reflects noise or artifacts in training data, which do not generalize
- Small train error, at cost of test high error
- Hence, predictions of overfitting models cannot be trusted but proper ML evaluation workflows should make it visible





# **UNDER- AND OVERFITTING IN REGRESSION**

- Poly-Regression, on data from sinusoidal function
- LM underfits, high-d overfits

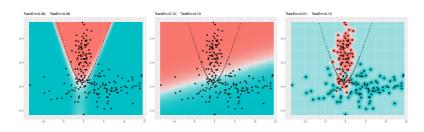




# **MATHEMATICAL DEFINITIONS**

- Nearly no reference does that, here is one approach
- Underfitting  $UF(\hat{f}, L) := GE(\hat{f}, L) GE(f^*, L)$ Diff in GE between  $\hat{f}$  and the Bayes optimal model
- Overfitting  $OF(\hat{f}, L) := GE(\hat{f}, L) \mathcal{R}_{emp}(\hat{f}, L)$ Diff between (theoretical) GE and training error





NB: Now, RHS is both UF and OF, let's say OF has "prio".

# OVERFITTING TRADE-OFFS

The potential for overfitting is influenced by:

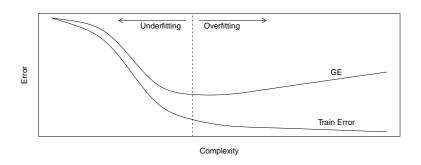
- Complexity of hypothesis space
- Amount of training data
- Dimensionality of feature space
- Irreducible noise

#### Implications:

- The larger / more complex is  $\mathcal{H}$ , the more data we need to tell candidate models apart
- The less data we have, the more we need to stick with "constrained"  $\mathcal{H}$
- OF can happen for LMs too: If feature space is very high-dim
- Tightly connected to the bias-var-noise decomposition of GE of a learner ( $\rightarrow$  which we study elsewhere).



# **COMPLEXITY VS GE**





- Common U-shape of GE if complexity or train-rounds go up.
- Optimal level of complexity:
  Simplest model for which GE is not significantly outperformed
- We could also call "Point of OF" the point where GE goes up.

#### **AVOIDING OVERFITTING**

- Use more or better data not always possible, but maybe can augment data, e.g., for images
- ullet Constrain  ${\mathcal H}$  directly by using less complex model classes
- Many learners come with HPs that can constrain complexity
- Use "early-stopping"
- Occam's razor in model selection: If GE not strongly reduced for more complex class, use the simpler model.

All of the above are methods of regularization, which we study in a dedicated chapter.

