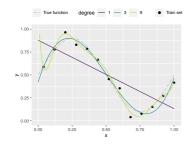
# **Introduction to Machine Learning**

# **Evaluation: Training Error**



#### Learning goals

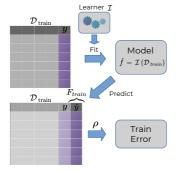
- Understand the definition of training error
- Understand why train error is unreliable for models of higher complexity when overfitting can occur

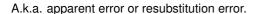


#### TRAINING ERROR

Simply plugin predictions for data that model has been trained on:

$$ho(\mathbf{y}_{ ext{train}}, oldsymbol{\mathcal{F}}_{ ext{train}})$$
 where  $oldsymbol{\mathcal{F}}_{ ext{train}} = egin{bmatrix} \hat{f}_{\mathcal{D}_{ ext{train}}}(\mathbf{x}_{ ext{train}}^{(1)}) \ & \dots \ & \hat{f}_{\mathcal{D}_{ ext{train}}}(\mathbf{x}_{ ext{train}}^{(m)}) \end{bmatrix}$ 



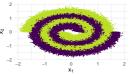




#### **EXAMPLE 1: KNN**

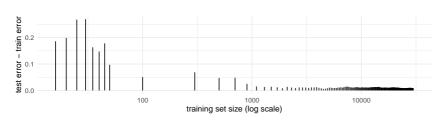
For large data, and some models, train error **can maybe** yield a good approximation of the GE:

- Use k-NN (k = 15).
- Up to 30K points from spirals to train.
- Use very large extra set for testing (to measure "true GE").



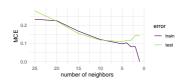


We increase train size, and see how gap between train error and GE closes.

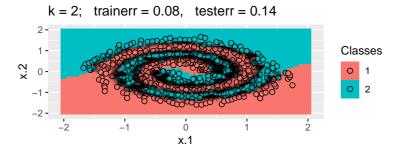


#### **EXAMPLE 1: KNN/2**

- Fix train size to 500 and vary k.
- Low train error for small k is deceptive.
   Model is very local and overfits.



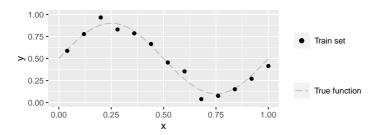




Black region are misclassifications from large test test.

## **EXAMPLE 2: POLYNOMIAL REGRESSION**

Sample data from  $0.5 + 0.4 \cdot \sin(2\pi x) + \epsilon$ 





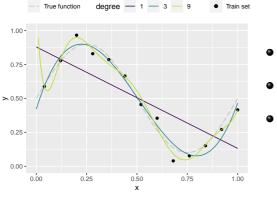
We fit a  $d^{th}$ -degree polynomial:

$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \theta_0 + \theta_1 \mathbf{x} + \dots + \theta_d \mathbf{x}^d = \sum_{j=0}^d \theta_j \mathbf{x}^j.$$

### **EXAMPLE 2: POLYNOMIAL REGRESSION / 2**

Simple model selection problem: Which *d*?

Visual inspection vs quantitative MSE on training set:



- d = 1: MSE = 0.036: clearly underfitting
- d = 3: MSE = 0.003: pretty OK
- d = 9: MSE = 0.001: clearly overfitting



Using the train error chooses overfitting model of maximal complexity.

#### TRAIN ERROR CAN EASILY BECOME 0

- For 1-NN it is always 0 as each  $\mathbf{x}^{(i)}$  is its own NN at test time.
- Extend any ML training in the following way: After normal fitting, we also store the training data. During prediction, we first check whether x is already stored in this set. If so, we replicate its label. The train error of such an (unreasonable) procedure will be 0.
- There are so called interpolators interpolating splines, interpolating Gaussian processes - whose predictions can always perfectly match the regression targets, they are not necessarily good as they will interpolate noise, too.



#### **CLASSICAL STATISTICAL GOF MEASURES**

- Goodness-of-fit measures like  $R^2$ , likelihood, AIC, BIC, deviance are all based on the training error.
- For models of restricted capacity, and enough data, and non-violated distributional assumptions: they might work.
- Hard to gauge when that breaks, for high-dim, more complex data.
- How do you compare to non-param ML-like models?



Out-of-sample testing is probably always a good idea!