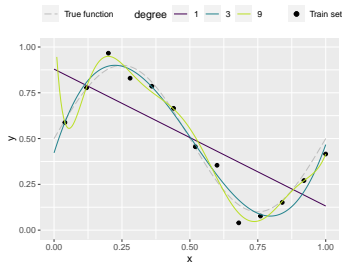


# Introduction to Machine Learning

## Evaluation Training Error



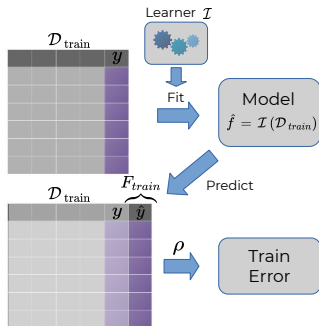
### Learning goals

- 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:

$$\rho(\mathbf{y}_{\text{train}}, \mathbf{F}_{\text{train}}) \text{ where } \mathbf{F}_{\text{train}} = \begin{bmatrix} \hat{f}_{\mathcal{D}_{\text{train}}}(\mathbf{x}_{\text{train}}^{(1)}) \\ \vdots \\ \hat{f}_{\mathcal{D}_{\text{train}}}(\mathbf{x}_{\text{train}}^{(m)}) \end{bmatrix}$$

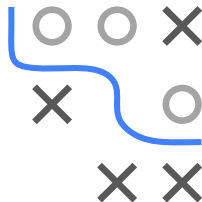
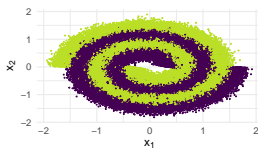


A.k.a. apparent error or resubstitution error.

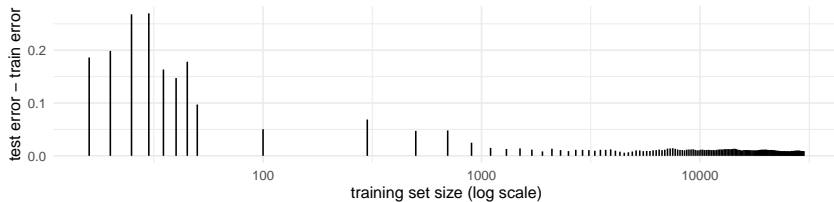
# EXAMPLE 1: KNN

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").

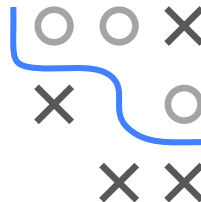
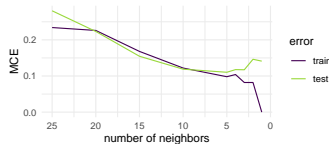


We increase train size, and see how gap between train error and GE closes.

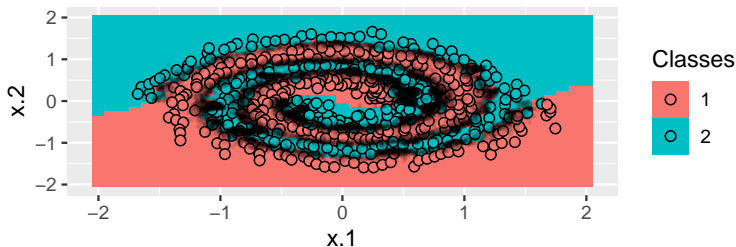


# EXAMPLE 1: KNN / 2

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



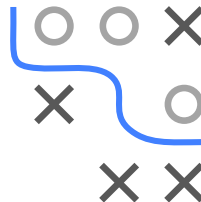
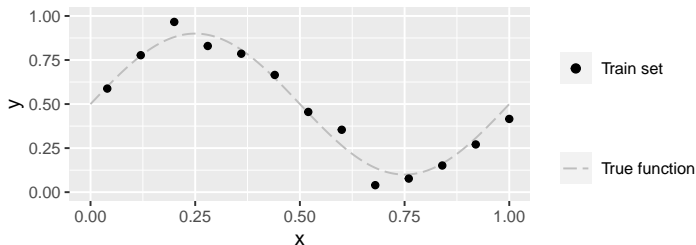
$k = 2$ ;  $\text{trainerr} = 0.08$ ,  $\text{testerr} = 0.14$



Black region are misclassifications from large test test.

# EXAMPLE 2: POLYNOMIAL REGRESSION

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



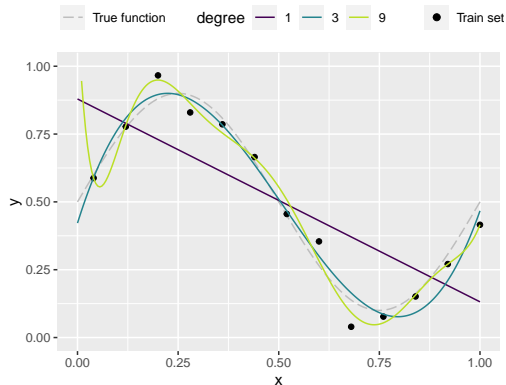
We fit a  $d^{th}$ -degree polynomial:

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

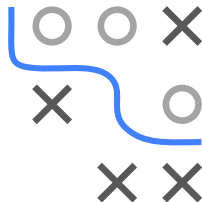
## EXAMPLE 2: POLYNOMIAL REGRESSION / 2

Simple model selection problem: Which  $d$ ?

Visual inspection vs quantitative MSE on training set:



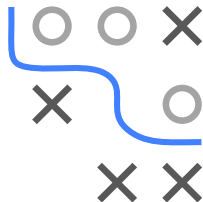
- $d = 1$ : MSE = 0.036:  
clearly underfitting
- $d = 3$ : MSE = 0.003:  
pretty OK
- $d = 9$ : MSE = 0.001:  
clearly overfitting



Using the train error chooses overfitting model of maximal complexity.

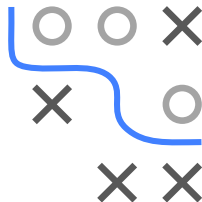
# TRAIN ERROR CAN EASILY BECOME 0

- 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!