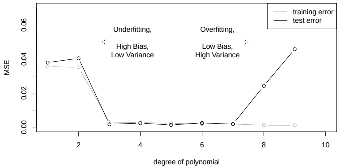
Introduction to Machine Learning

Evaluation: Test Error



Learning goals

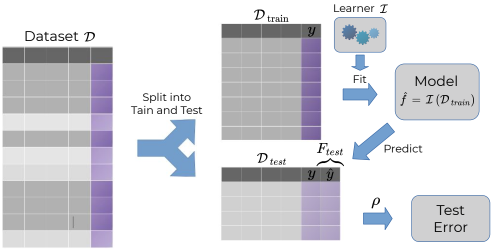
- Understand the definition of test error
- Understand that test error is more reliable than train error
- Bias-Variance analysis of holdout splitting

TEST ERROR AND HOLD-OUT SPLITTING

- Simulate prediction on unseen data, to avoid optimistic bias:

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

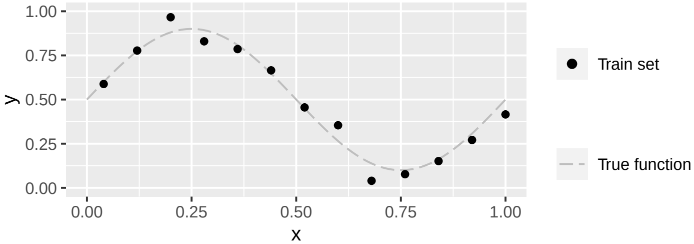
- Partition data, e.g., 2/3 for train and 1/3 for test.



A.k.a. holdout splitting.

EXAMPLE: POLYNOMIAL REGRESSION

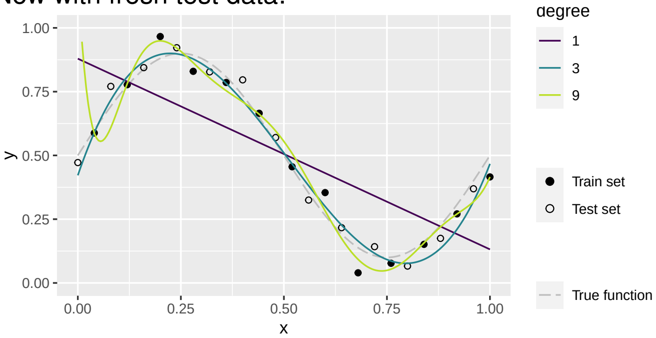
Previous example:



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

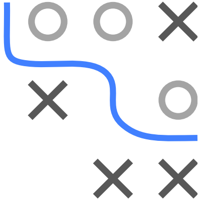
EXAMPLE: POLYNOMIAL REGRESSION / 2

Now with fresh test data:



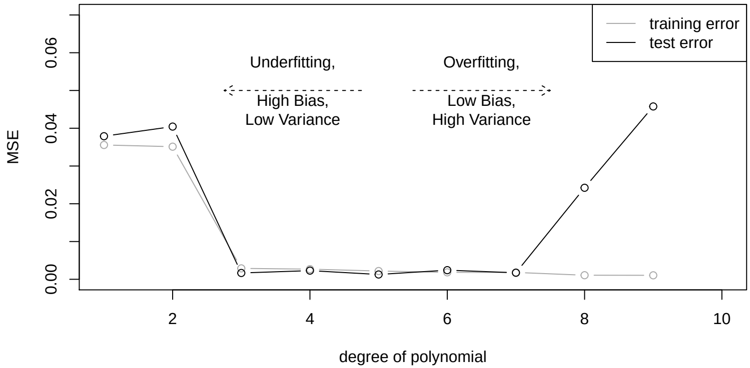
- $d = 1$: MSE = 0.038: clearly underfitting
- $d = 3$: MSE = 0.002: pretty OK
- $d = 9$: MSE = 0.046: clearly overfitting

While train error monotonically decreases in d, test error shows that high-d polynomials overfit.



TEST ERROR

Let's plot train and test MSE for all d:



Increasing model complexity tends to cause

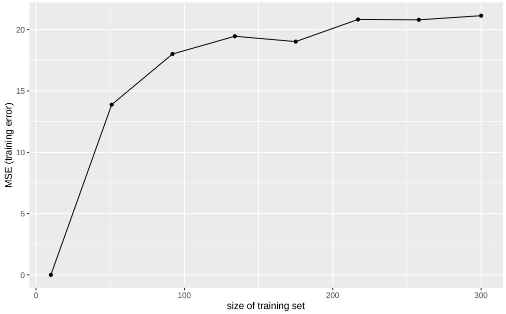
- a decrease in training error, and
- a U-shape in test error
  (first underfit, then overfit, sweet-spot in the middle).

TRAINING VS. TEST ERROR

- Boston Housing data
- Polynomial regression (without interactions)

The training error...

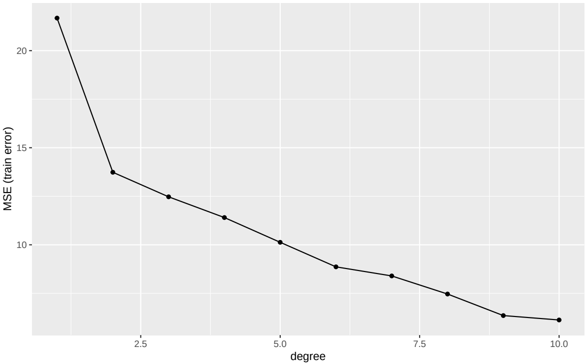
- decreases with smaller training set size as it becomes easier for the model to learn all observed patterns perfectly.



TRAINING VS. TEST ERROR / 2

The training error...

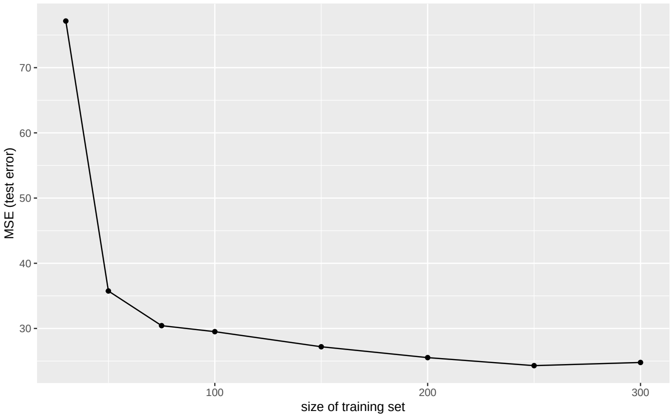
- decreases with increasing model complexity as the model gets better at learning more complex structures.

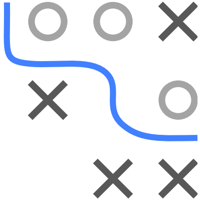


TRAINING VS. TEST ERROR / 3

The test error...

- will typically decrease with larger training set size as the model generalizes better with more data to learn from.

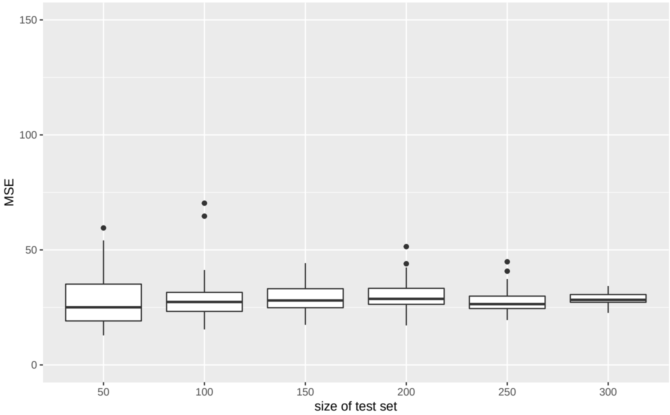




TRAINING VS. TEST ERROR / 4

The test error...

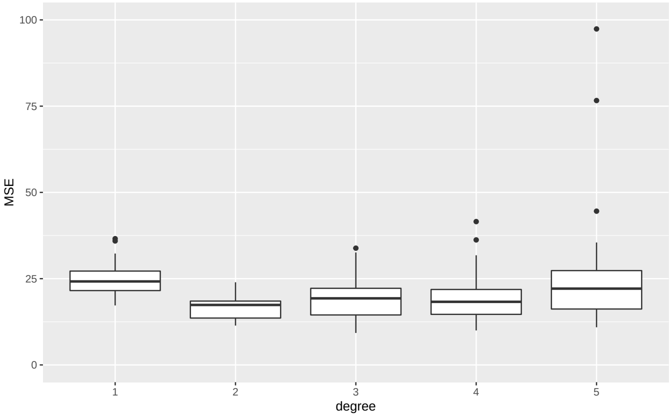
- will have higher variance with smaller test set size.



TRAINING VS. TEST ERROR / 5

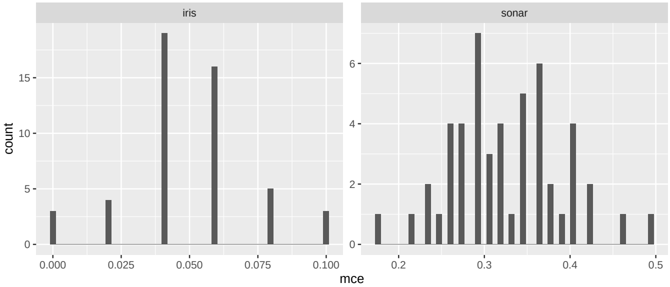
The test error...

- will have higher variance with increasing model complexity.



BIAS AND VARIANCE

- Test error is a good estimator of GE, given a) we have enough data b) test data is representative i.i.d.
- Estimates for smaller test sets can fluctuate considerably – this is why we use resampling in such situations.
  Repeated $\frac{2}{3}$ / $\frac{1}{3}$ holdout splits:
  `iris` ($n = 150$) and `sonar` ($n = 208$).



BIAS-VARIANCE OF HOLD-OUT – EXPERIMENT

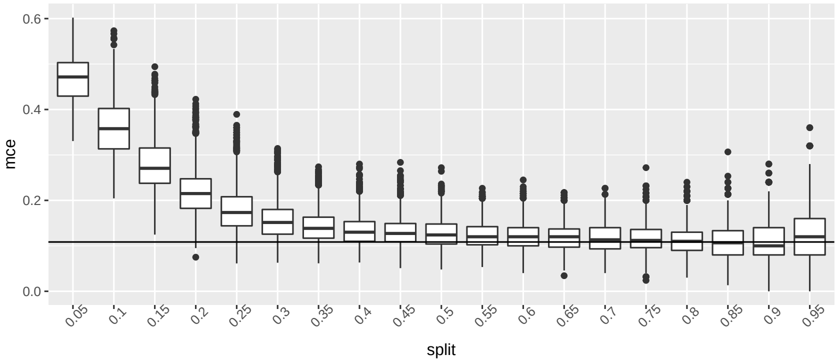
Hold-out sampling produces a trade-off between **bias** and **variance** that is controlled by split ratio.

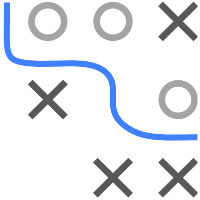
- Smaller training set $\rightarrow$ poor fit, pessimistic bias in $\widehat{\mathrm{GE}}$.
- Smaller test set $\rightarrow$ high variance.

Experiment:

- `spirals` data ($sd = 0.1$), with CART tree.
- Goal: estimate real performance of a model with $|\mathcal{D}_{\text{train}}| = 500$.
- Split rates $s \in \{0.05, 0.10, ..., 0.95\}$ with $|\mathcal{D}_{\text{train}}| = s \cdot 500$.
- Estimate error on $\mathcal{D}_{\text{test}}$ with $|\mathcal{D}_{\text{test}}| = (1 - s) \cdot 500$.
- 50 repeats for each split rate.
- Get "true" performance by often sampling 500 points, fit learner, then eval on 10^5 fresh points.

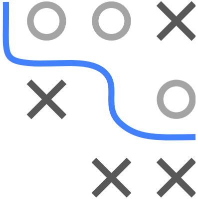
BIAS-VARIANCE OF HOLD-OUT – EXPERIMENT / 2





- Clear pessimistic bias for small training sets – we learn a much worse model than with 500 observations.
- But increase in variance when test sets become smaller.

BIAS-VARIANCE OF HOLD-OUT – EXPERIMENT / 3



- Let's now plot the MSE of the holdout estimator.
- NB: Not MSE of model, but squared difference between estimated holdout values and true performance (horiz. line in prev. plot).
- Best estimator is ca. train set ratio of 2/3.
- NB: This is a single experiment and not a scientific study, but this rule-of-thumb has also been validated in larger studies.