

AutoML: Evaluation

Evaluation of ML Models (Review)

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Introduction

- Performance estimation of a model** Estimate generalization error of a model on new (unseen) data, drawn from the same data generating process.
- Performance estimation of an algorithm** Estimate generalization error of a learning algorithm, trained on a data set of a certain size, on new (unseen) data, all drawn from the same data generating process.
- Model selection** Select the best model from a set of potential candidate models (e.g., different model classes, different hyperparameter settings, different feature sets).

Performance Evaluation

ML performance evaluation provides clear and simple protocols for reliable model validation.

- often simpler than classical statistical model diagnosis
- relies only on few assumptions
- still hard enough and offers **lots** of options to cheat and make mistakes

Performance Measures

We measure performance using a statistical estimator for the **generalization error** (GE).

GE = expected loss of a fixed model

\hat{GE} = estimated loss averaged across finite sample

Example: Mean squared error (L2 loss)

$$\hat{GE} = MSE = \frac{1}{n} \sum_{i=1}^n \left(y^{(i)} - \hat{y}^{(i)} \right)^2$$

Measures: Inner vs. Outer Loss

Inner loss = loss used in learning (training)

Outer loss = loss used in evaluation (testing)
= evaluation measure

Optimally: inner loss = outer loss

Not always possible:

some losses are hard to optimize or no loss is specified directly

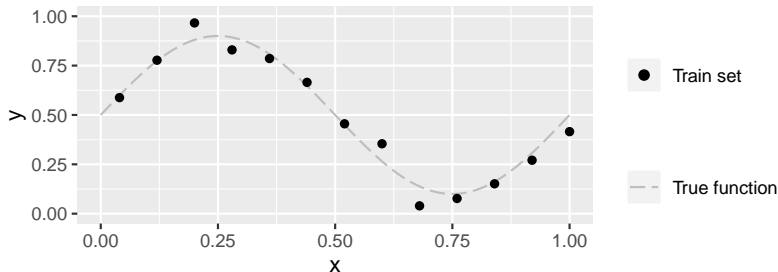
Example:

Logistic Regression → minimize binomial loss

kNN → no explicit loss minimization

Inner Loss Example: Polynomial Regression I

Sample data from sinusoidal function $0.5 + 0.4 \cdot \sin(2\pi x) + \epsilon$ with measurement error ϵ .

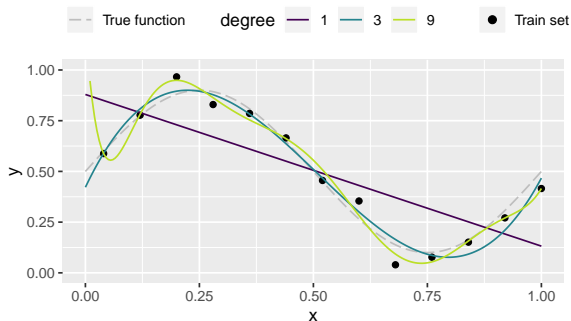


Assume data generating process unknown. Approximate with d th-degree polynomial:

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

Inner Loss Example: Polynomial Regression II

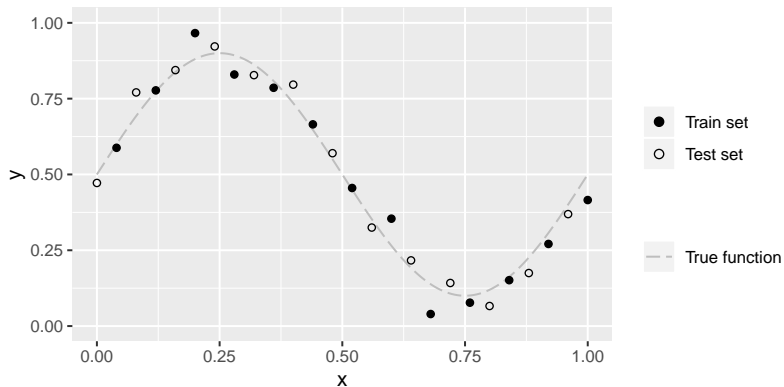
How should we choose d ?



$d=1$: $MSE = 0.036$ – clear underfitting, $d=3$: $MSE = 0.003$ – ok?, $d=9$: $MSE = 0.001$ – clear overfitting

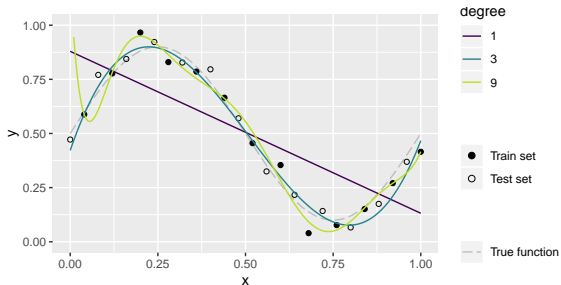
Simply using the training error seems to be a bad idea.

Outer Loss Example: Polynomial Regression I



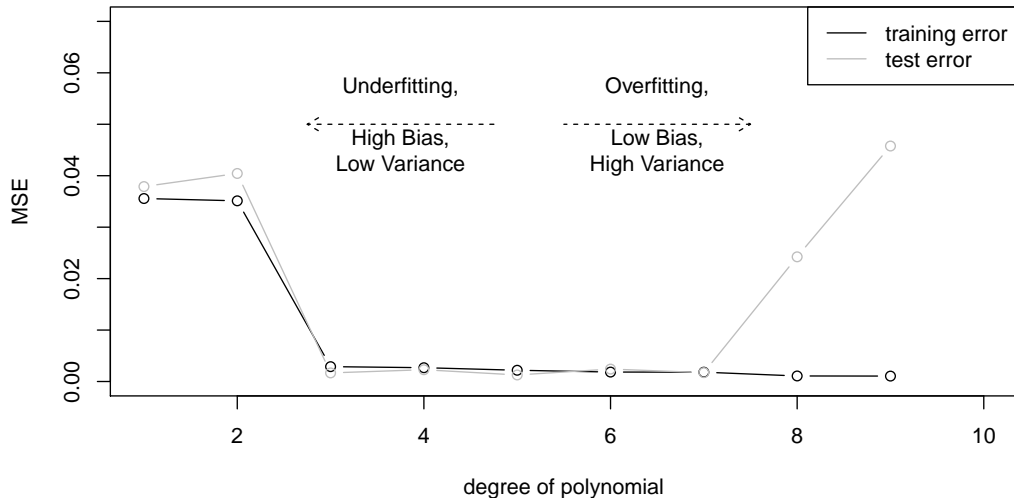
Outer Loss Example: Polynomial Regression II

How should we choose d ?

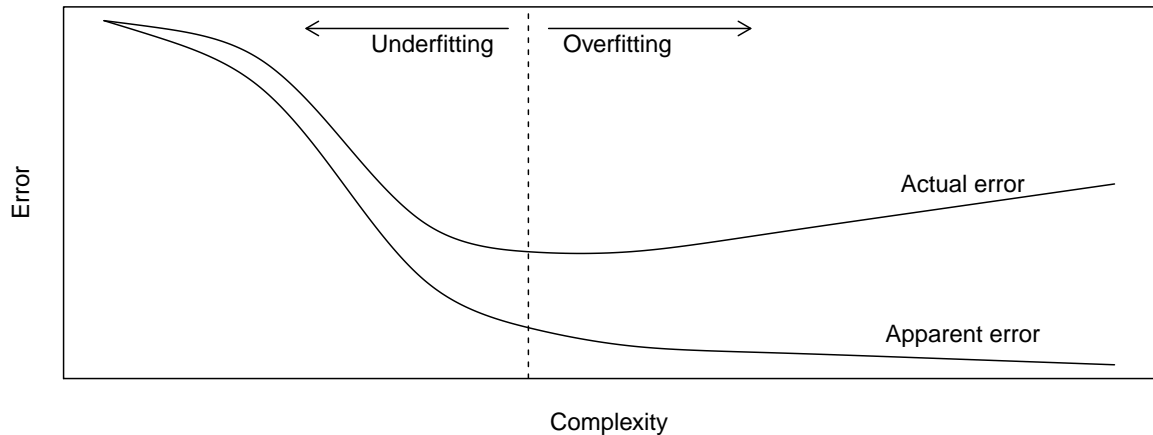


$d=1$: $\text{MSE} = 0.038$ – clear underfitting, $d=3$: $\text{MSE} = 0.002$ – ok?, $d=9$: $\text{MSE} = 0.046$ – clear overfitting

Outer Loss Example: Polynomial Regression III



General Trade-Off Between Error and Complexity



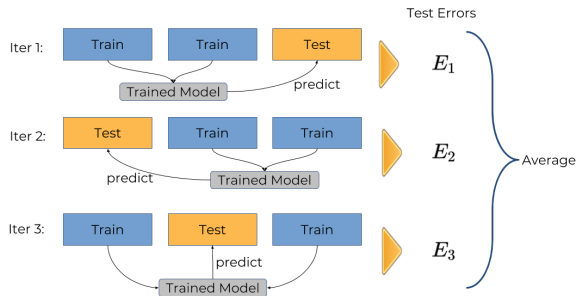
Resampling

- uses data efficiently
- repeatedly split in train and test, average results
- make training sets large (to keep the pessimistic bias small), reduce variance introduced by smaller test sets through many repetitions and averaging of results

Cross-Validation

- split data into k roughly equally-sized partitions
- use each part as test set and join the $k - 1$ others for training, repeat for all k combinations
- obtain k test errors and average

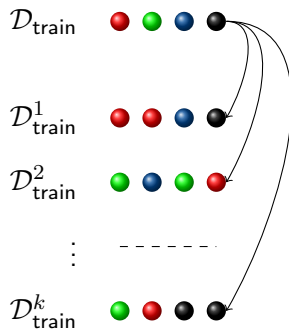
Example 3-fold cross-validation:



10-fold cross-validation is common.

Bootstrap

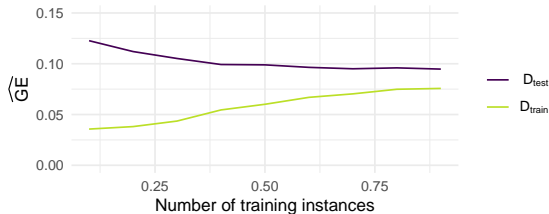
- randomly draw k training sets of size n with replacement from the data
- evaluate on observations from the original data that are not in the training set
- obtain k test errors and average



Training sets will contain about 63.2% of observations on average.

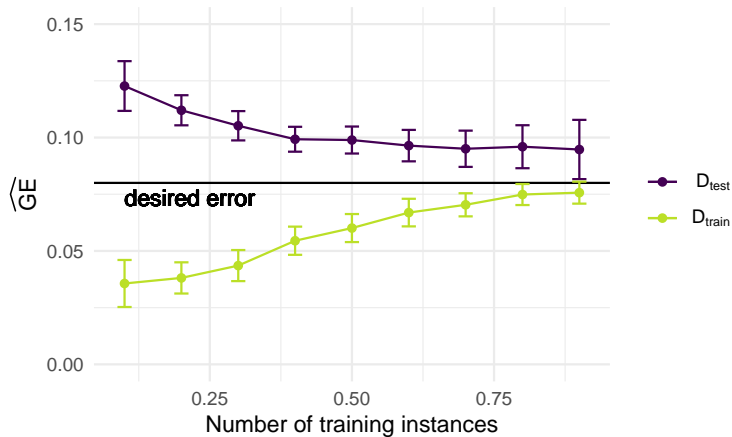
Learning Curves I

- compares performance of a model on training and test data over a varying number of training instances → how fast can a learner learn the given relationship in the data?
- can also be over number of iterations of a learner (e.g. epochs in deep learning), or AutoML system over time
- learning usually fast in the beginning
- visualizes when a learner has learned as much as it can:
 - ▶ when performance on training and test set reach a plateau
 - ▶ when gap between training and test error remains the same



Learning Curves II

Ideal learning curve:

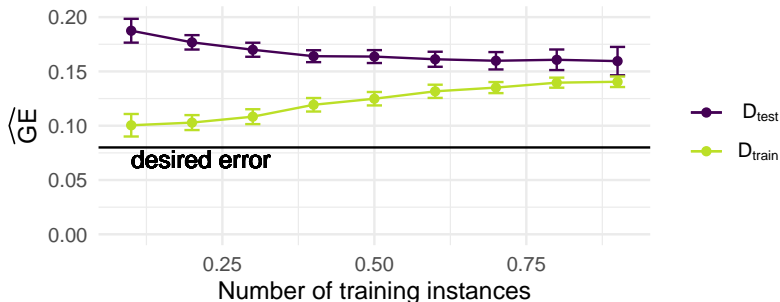


Learning Curves III

In general, there are two reasons for a bad learning curve:

① high bias in model/underfitting

- ▶ training and test errors converge at a high value
- ▶ model can't learn underlying relationship and has high systematic errors, no matter how big the training set
- ▶ poor fit, which also translates to high test error



Learning Curves IV

② high variance in model/overfitting

- ▶ large gap between training and test errors
- ▶ model requires more training data to improve
- ▶ model has a poor fit and does not generalize well

