QTM 347 Machine Learning

Lecture 6: Cross-Validation

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Suggested reading: ISL Chapter 5

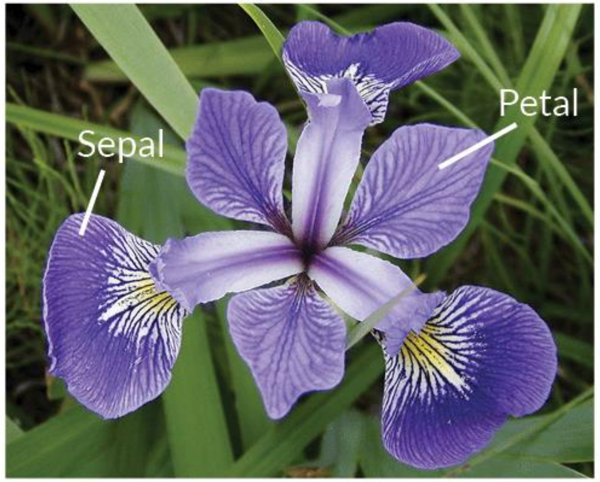
EMORY

Lecture plan

- Review of LDA and QDA

- Cross validation

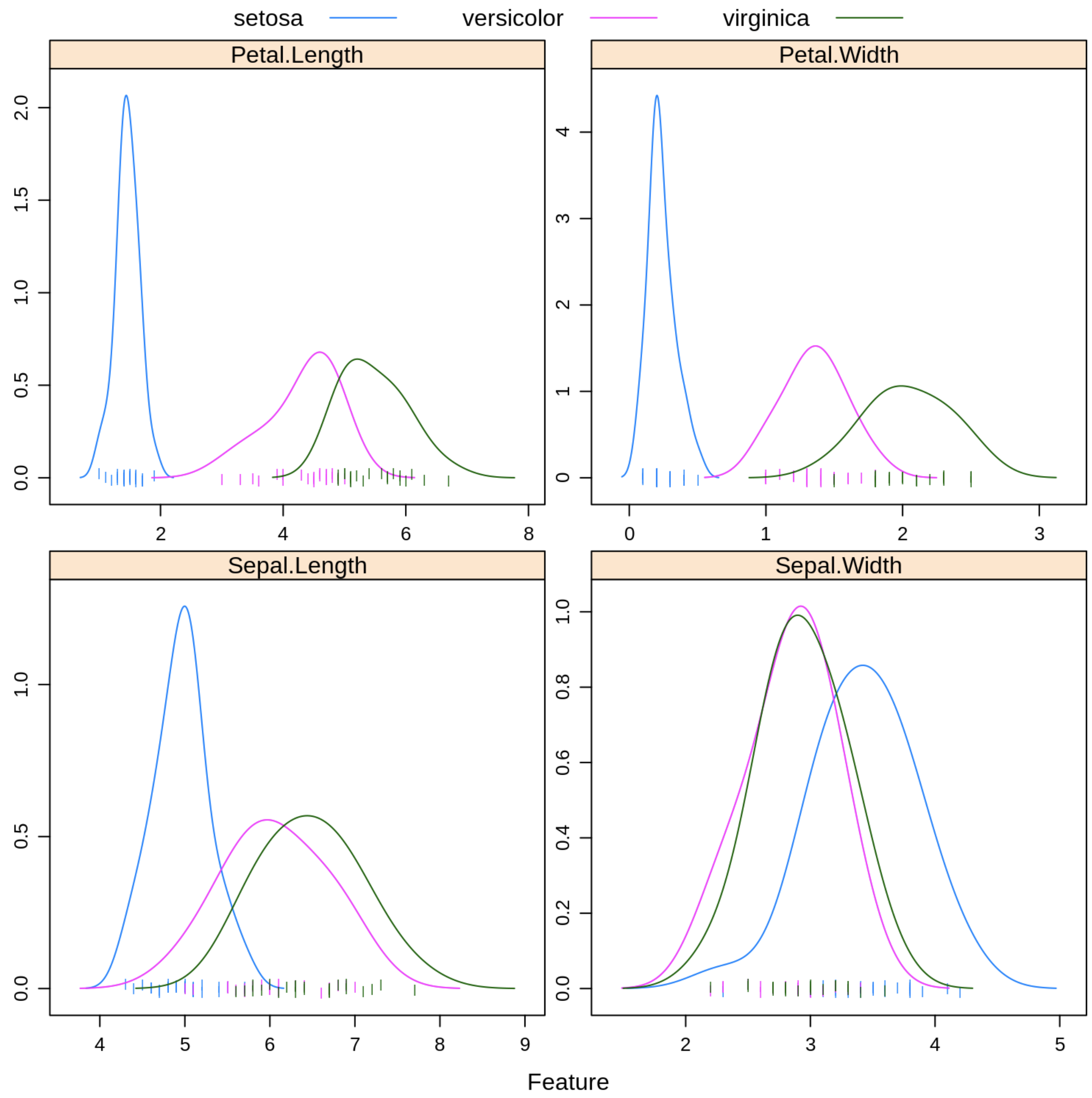
Example of LDA/QDA: An iris data set



Iris Versicolor

Iris Setosa

Iris Virginica



LDA

- For each class k, we model $P(X = x|Y = k) = f_k(x)$ as a *Multivariate Normal Distribution* $N(\mu_k, \Sigma)$ with mean μ_k and covariance matrix Σ
- We estimate $\hat{P}(X = x|Y = k)$ as $N(\hat{\mu}_k, \hat{\Sigma})$ and $\hat{P}(Y = k) = \hat{\pi}_k$
- We apply to Bayes theorem to obtain $P(Y = k \mid X = x)$

$$\hat{P}(Y = k \mid X = x) = \frac{\hat{P}(Y = k, X = x)}{\hat{P}(X = x)} = \frac{\hat{P}(X = x \mid Y = k)\hat{P}(Y = k)}{\sum_j \hat{P}(X = x \mid Y = j)\hat{P}(Y = j)}$$

QDA

- For each class k, we model $P(X = x|Y = k) = f_k(x)$ as a *Multivariate Normal Distribution* $N(\mu_k, \Sigma_k)$ with mean μ_k and covariance matrix Σ_k

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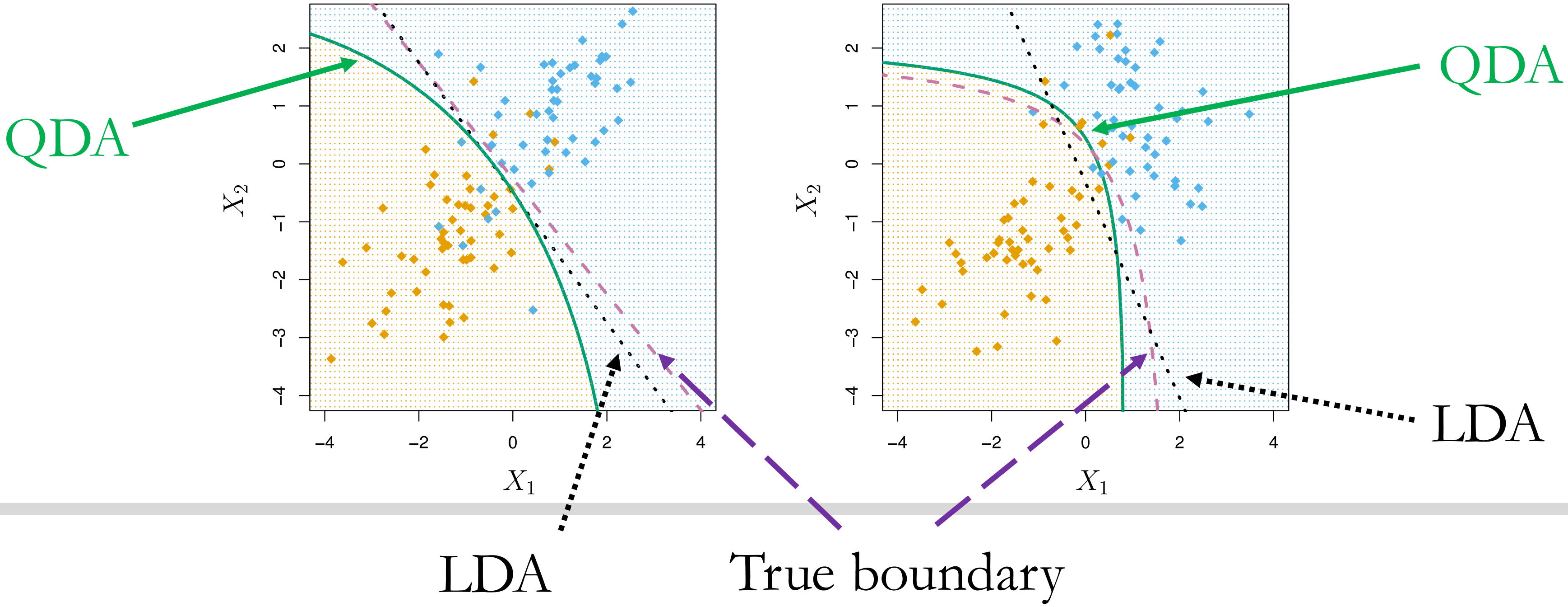
Comparison between LDA and QDA

- **Decision boundary**: the set of points in which 2 classes do just as well
  - LDA has *linear* decision boundary
  - QDA has *quadratic* decision boundary
- **Bias-variance tradeoff**
  - LDA is less flexible but has a smaller variance. Small sample size n: LDA
  - QDA requires more parameters. Large sample size n: QDA



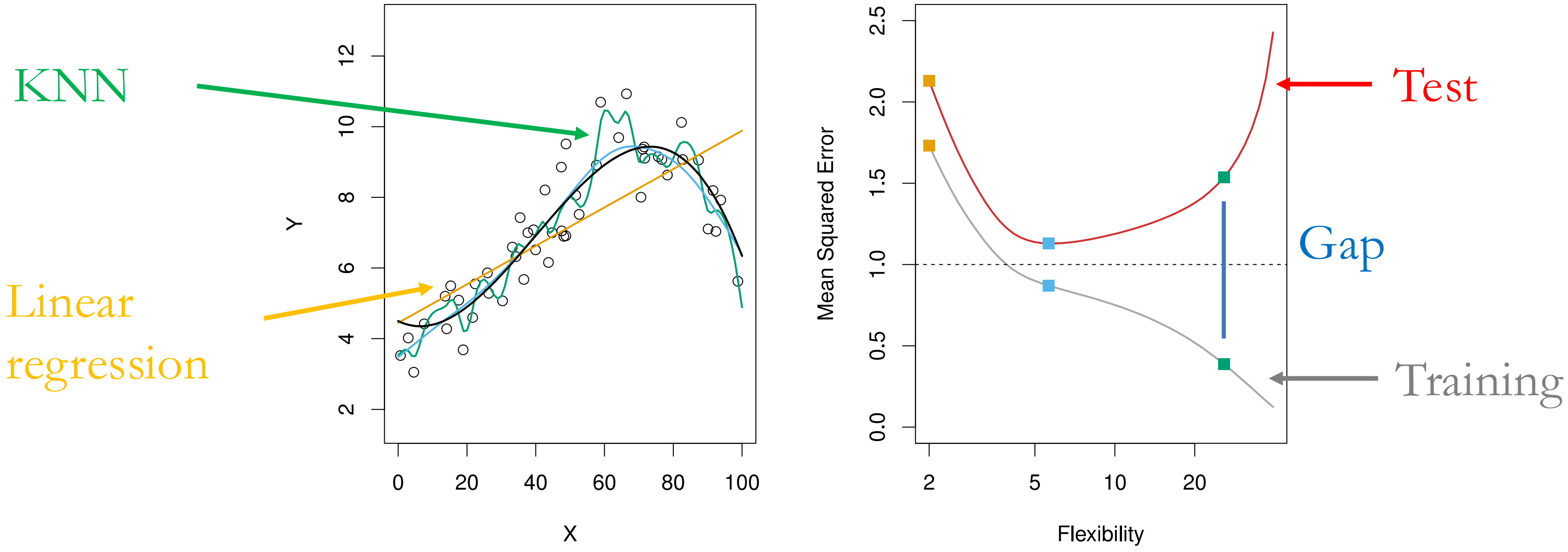
Lecture plan

- Review of LDA and QDA

- Cross validation

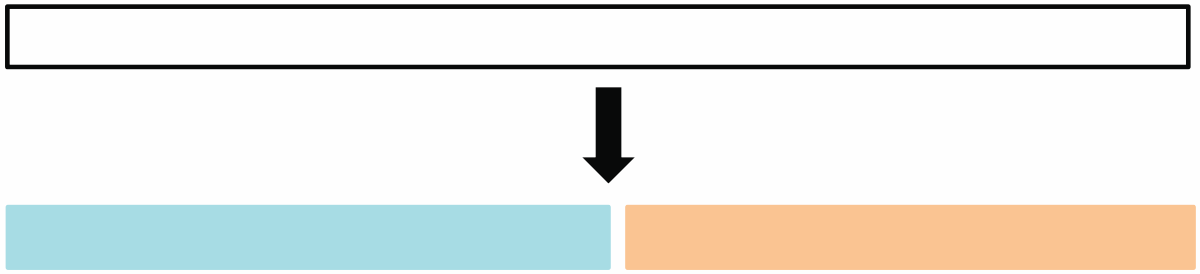
Motivation

- **Supervised learning**: Minimize test error
  - However, we only have access to the training error
  - There is often a gap between them
- **Illustration**: Suppose we know what f is (the black curve)
  - We generate data according to f as simulated data (in circles)



Validation set approach

- **Goal of validation set approach**: Using the training data set alone, find out the test error as closely as possible
- **A first attempt**:
  - Randomly split the data in two parts
  - Train the method in the first part
  - Compute the error on the second part



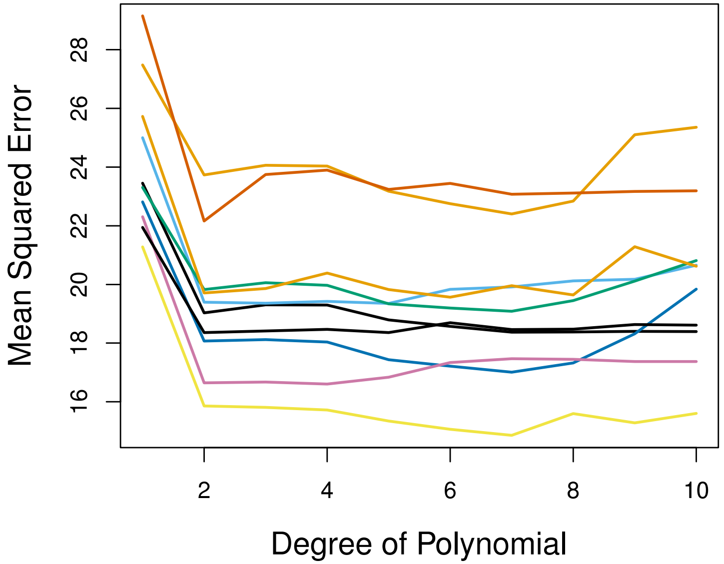
EMORY

Example

- Estimate miles per gallon (mpg) from engine horsepower
  - Auto data: horsepower, gas mileage, and other information for 392 vehicles
- **Simple linear regression**
  - $\text{mpg} = \beta_0 + \beta_1 \text{horsepower}$
- **Multiple linear regression with polynomial features**
  - $\text{mpg} = \beta_0 + \beta_1 \text{horsepower} + \beta_2 \text{horsepower}^2$
  - $\text{mpg} = \beta_0 + \beta_1 \text{horsepower} + \beta_2 \text{horsepower}^2 + \beta_3 \text{horsepower}^3$
- **Which polynomial is the right relationship?**
  - **Resampling**
    - Partition 392 samples into two sets with equal size
    - One is the training set and the other one is the validation set

Example

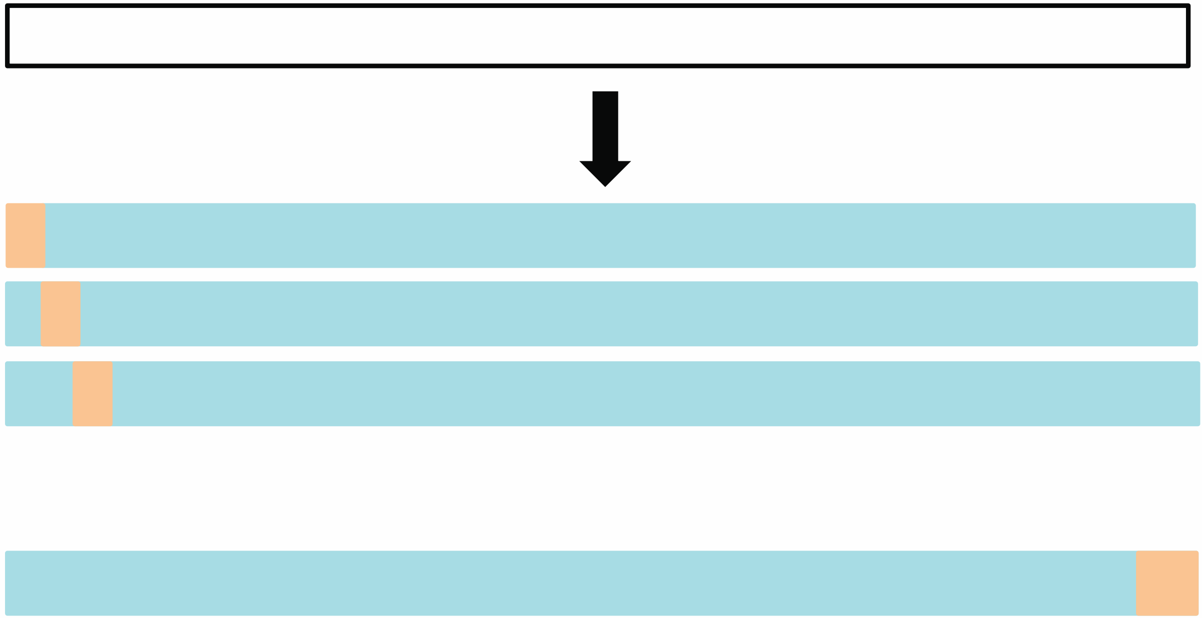
- Estimate miles per gallon (mpg) from engine horsepower



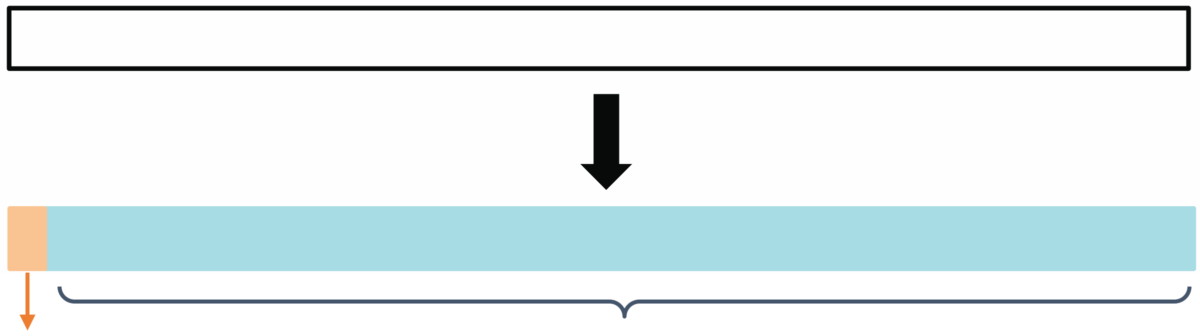
- Each line is the result with a different random split of the data into two parts
- Every split yields a different estimate of the error ☹

Leave-one-out cross-validation

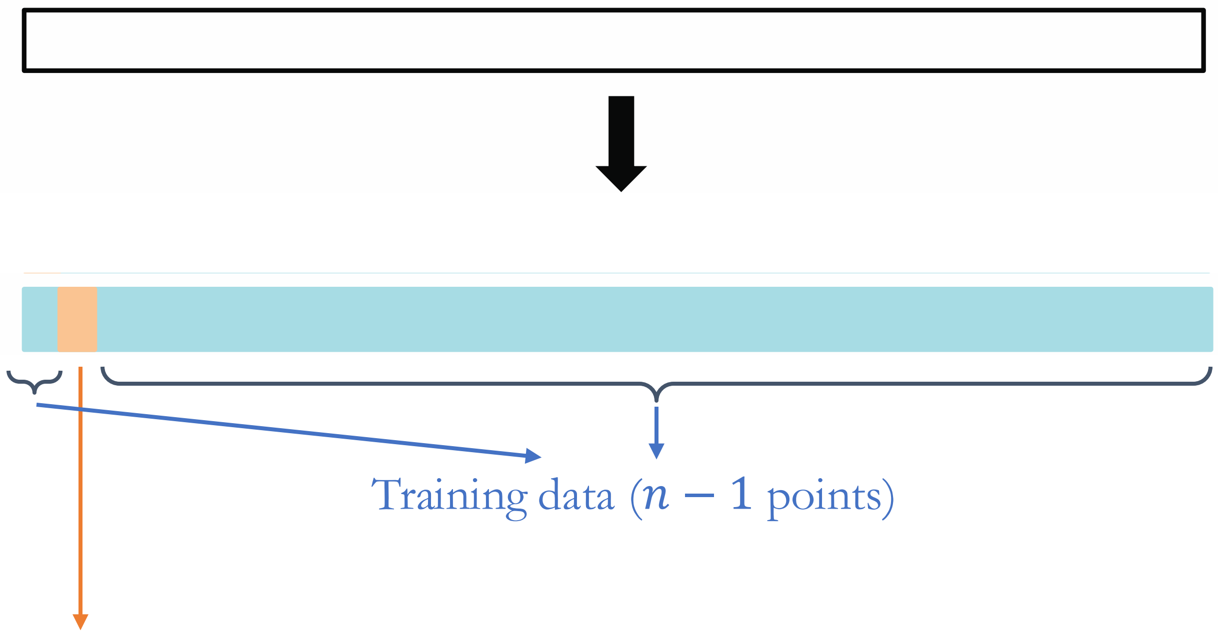
- **Leave-one-out cross-validation**
- For every $i = 1, \cdots, n$,
  - Train the model on every point except i;
  - Compute the test error on the hold-out point;
  - Average over all n points.



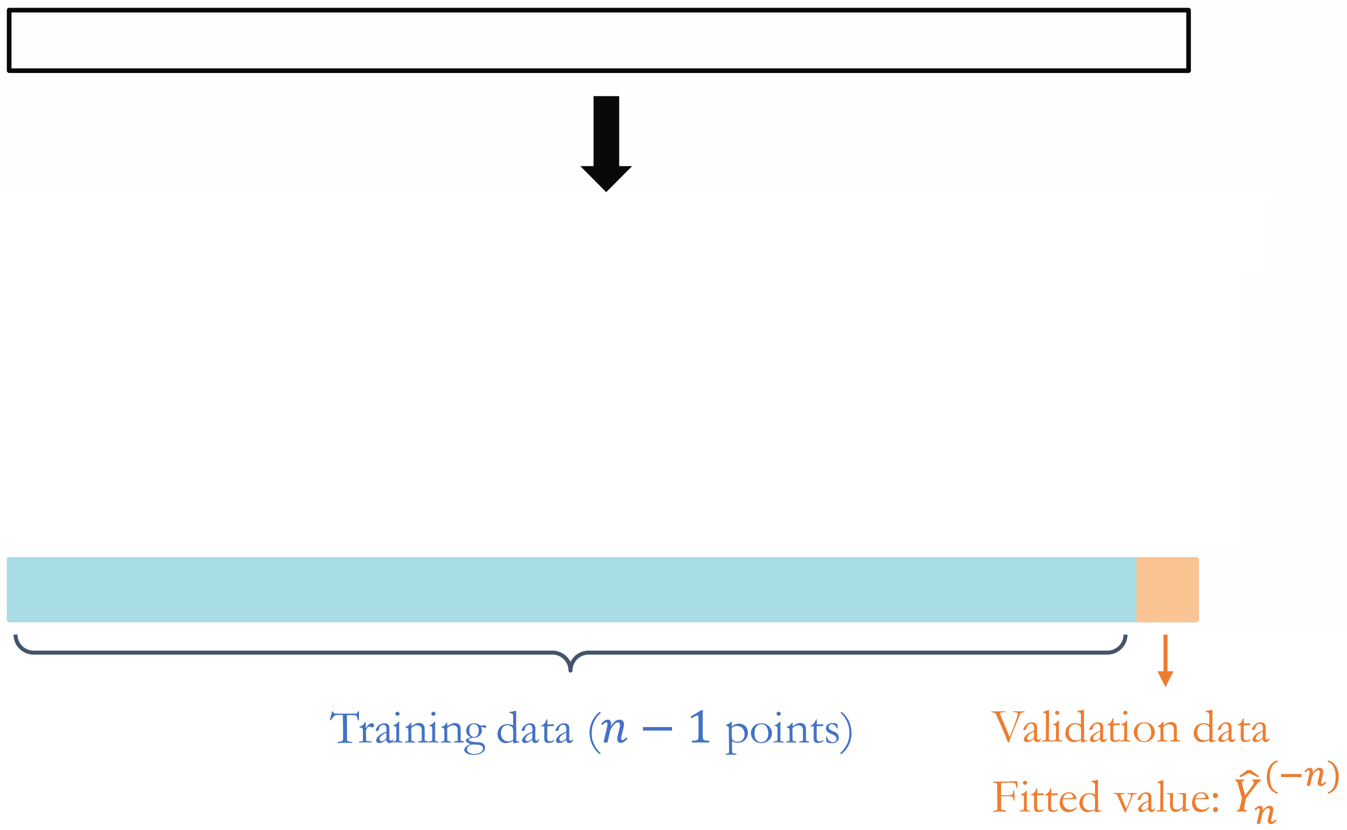
Leave-one-out cross-validation



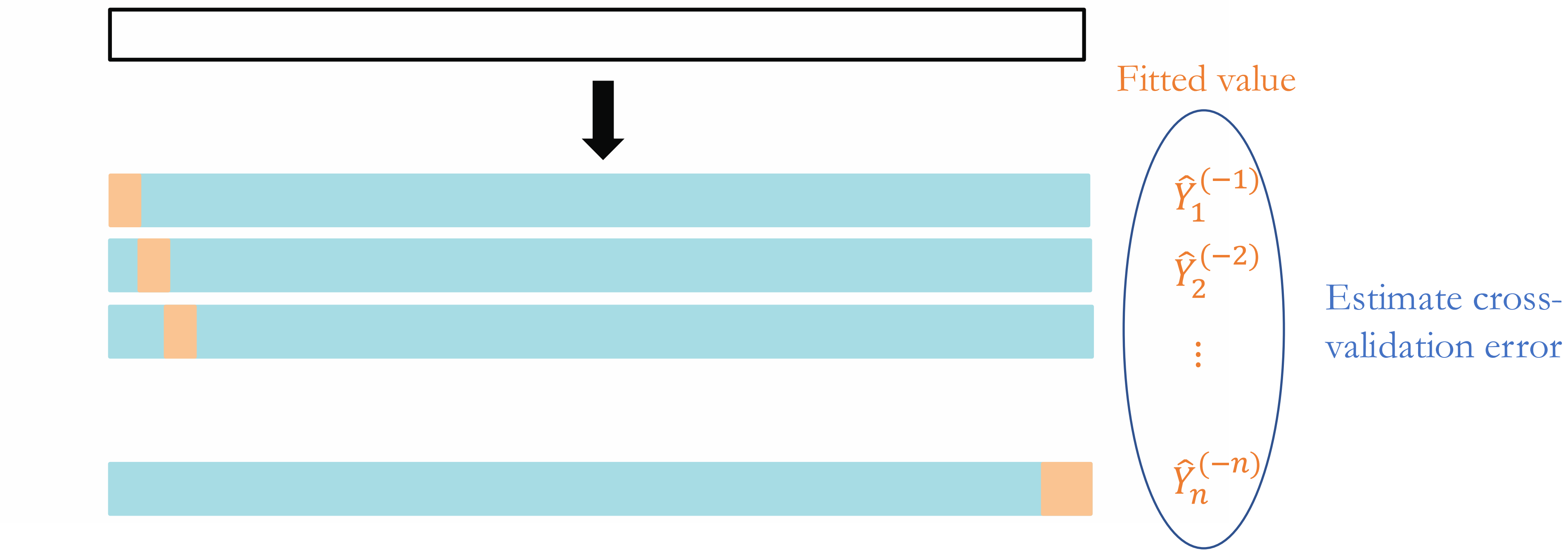
Leave-one-out cross-validation



Leave-one-out cross-validation



Leave-one-out cross-validation

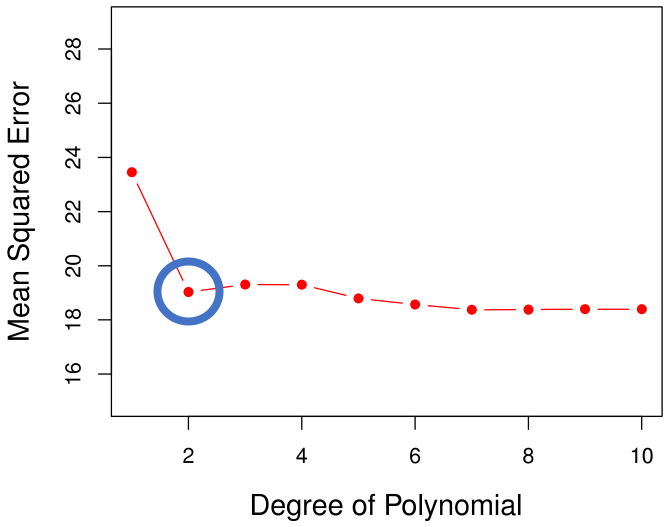


Cross-validation error

- **Regression** with mean squared loss
  - $\hat{Y}_i^{(-i)}$: Prediction for the ith sample without using the ith sample
  - $CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i^{(-i)})^2$
- **Classification** with zero-one loss
  - $\hat{Y}_i^{(-i)}$: Prediction for the ith sample without using the ith sample
  - $CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n} 1\left[Y_i \neq \hat{Y}_i^{(-i)}\right]$

Example

- Estimate miles per gallon (mpg) from engine horsepower
- The LOOCV error curve



LOOCV has low bias and no randomness

- Each training set in LOOCV has $n - 1$ observations, almost as many as are in the entire data set
  - LOOCV tends not to overestimate the test error rate by too much (low bias)
  - There is no randomness in the training/validation set splits

Computational concerns

- Computing $CV_{(n)}$ can be computationally expensive, since it involves fitting the model n times

- What if we use a model other than linear or polynomial regression?

- k-fold cross-validation: Split the data into k equal sized subsets
  - Only requires fitting the model k times
  - $\frac{n}{k}$ times speed up over leave one out cross-validation