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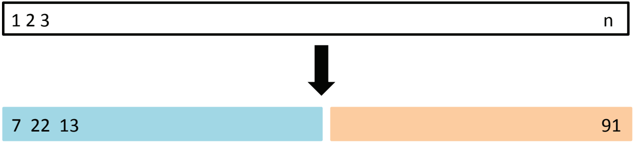

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- Split the data in two parts.
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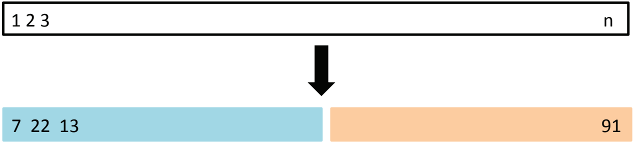

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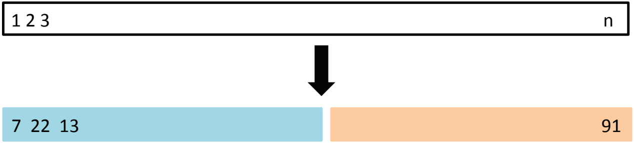
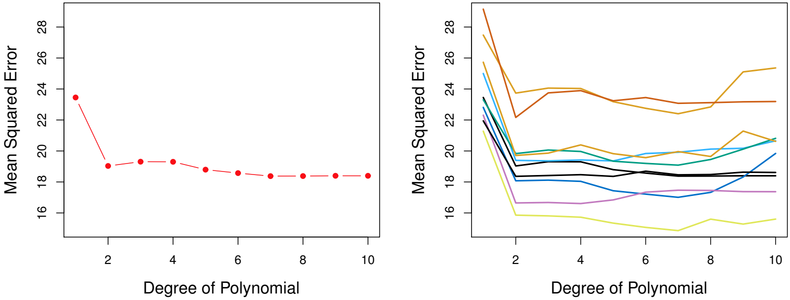


Validation set approach

Polynomial regression to estimate `mpg` from `horsepower` in the Auto data.



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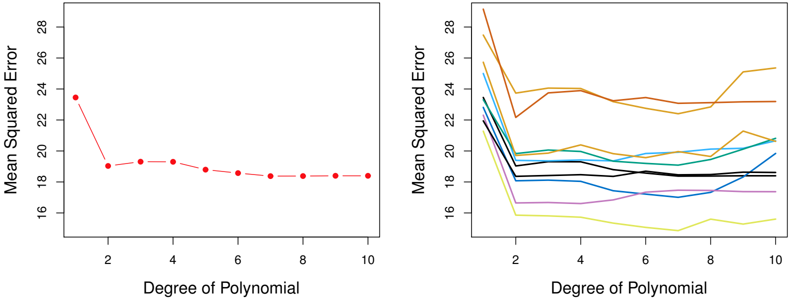
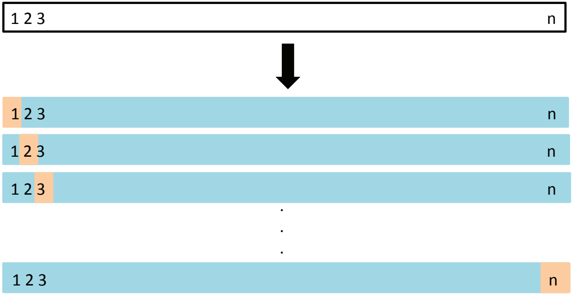


Problem: Every split yields a different estimate of the error.

Leave one out cross-validation

- For every $i = 1, \ldots, n$:
  - train the model on every point except i,
  - compute the test error on the held out point.



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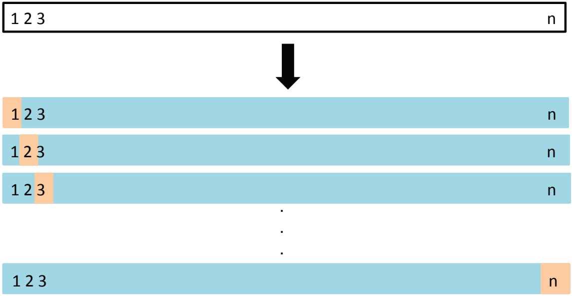

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$$\mathrm{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i^{(-i)})^2$$

Prediction for the i sample without using the ith sample.

Leave one out cross-validation

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$$\mathsf{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \mathbf{1}(y_i \neq \hat{y}_i^{(-i)})$$

... for a classification problem.

Leave one out cross-validation

Computing $\mathsf{CV}_{(n)}$ can be computationally expensive, since it involves fitting the model n times.

Leave one out cross-validation

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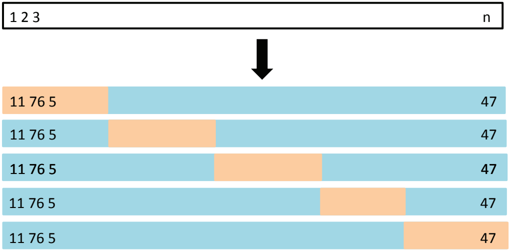
For linear regression, there is a shortcut:

$$\mathsf{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_{ii}}\right)^2$$

where h_{ii} is the leverage statistic.

k-fold cross-validation

- Split the data into k subsets or *folds*.



k-fold cross-validation

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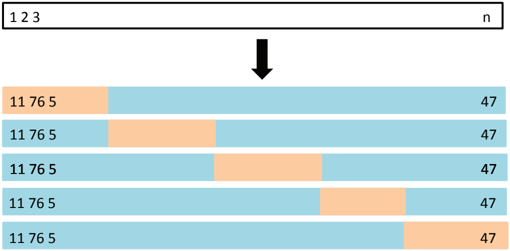

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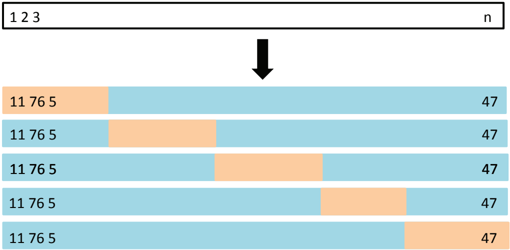
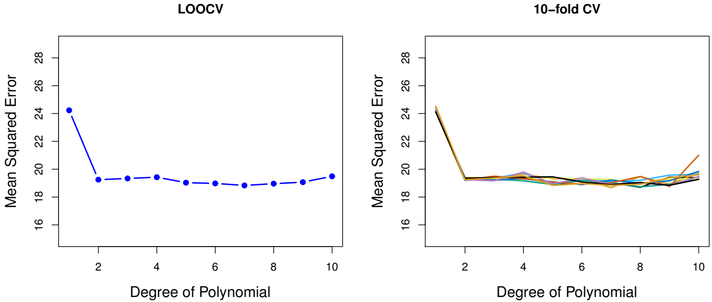
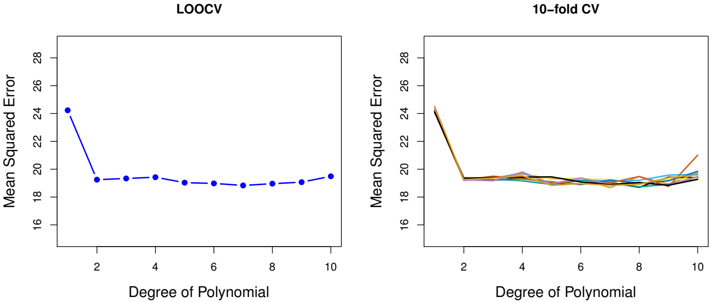


LOOCV vs. k-fold cross-validation

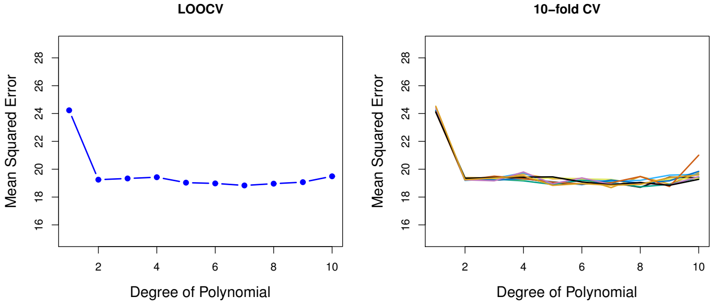


LOOCV vs. k-fold cross-validation



- k-fold CV depends on the chosen split (somewhat).

LOOCV vs. k-fold cross-validation



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- In k-fold CV, we train the model on less data than what is available. This introduces **bias** into the estimates of test error.

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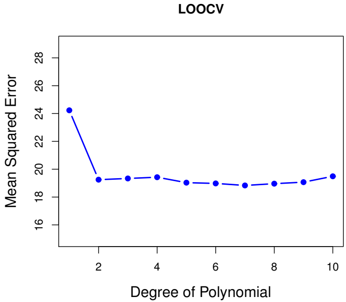

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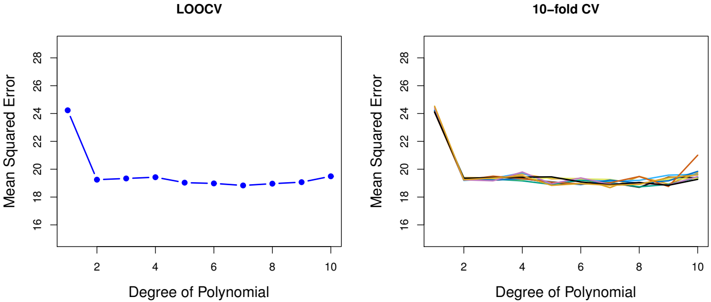
LOOCV vs. k-fold cross-validation



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- n-fold CV is equivalent LOOCV.