Module 3: Unsupervised learning, support vector machines and resampling

Principal Component Analysis, Clustering Algorithms, practical issues in clustering, support vector classifiers and support vector machines, **resampling methods: cross-validation and bootstrapping**

Reference: James, G., Witten, D., Hastie, T., Tibshirani, R. (2017). An Introduction to Statistical Learning: with Applications in R., Springer.)

Resampling Methods

- Resampling methods are an indispensable tool in modern statistics.
- They involve repeatedly drawing samples from a training set and refitting a model of interest on each sample in order to obtain additional information about the fitted model.
- For example, in order to estimate the variability of a linear regression fit, we can repeatedly draw different samples from the training data, fit a linear regression to each new sample, and then examine the extent to which the resulting fits differ.

Resampling Methods

Most commonly used resampling methods:

1. cross-validation
2. bootstrap

Resampling Methods

- cross-validation can be used to estimate the test error associated with a given statistical learning method in order to evaluate its performance, or to select the appropriate level of flexibility
- The process of evaluating a model's performance is known as model assessment
- The process of selecting the proper level of flexibility for a model is known as model selection
- The bootstrap is used in several contexts, most commonly to provide a measure of accuracy of a parameter estimate or of a given statistical learning method

Cross-Validation

- Test error rate
  - The test error is the average error that results from using a statistical learning method to predict the response on a new observation
- Training error rate

Validation set approach

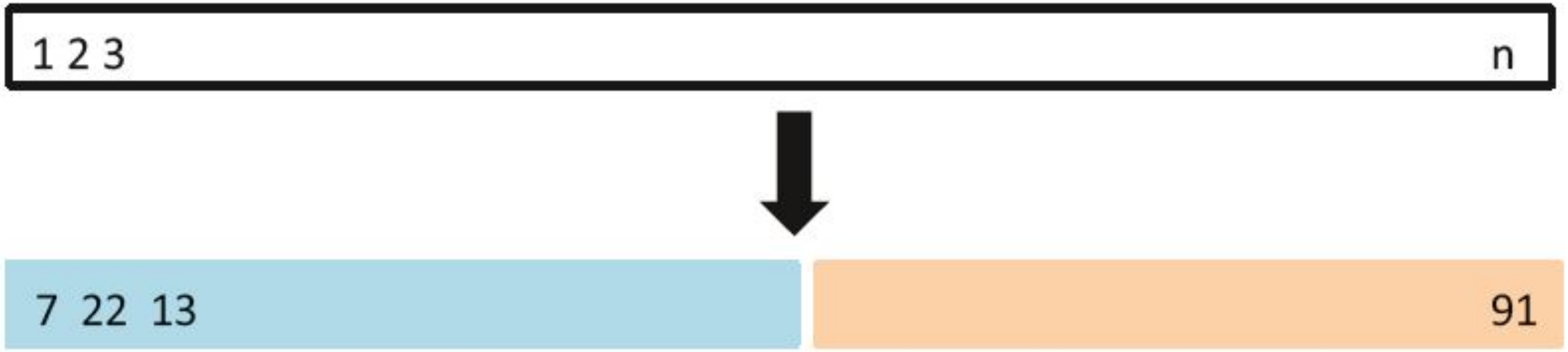


FIGURE 5.1. *A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.*

- It involves randomly dividing the available set of observations into two parts, a **training set** and a **validation set** or **hold-out set**
- The resulting validation set error rate—typically assessed using MSE in the case of a quantitative response—provides an estimate of the test error rate

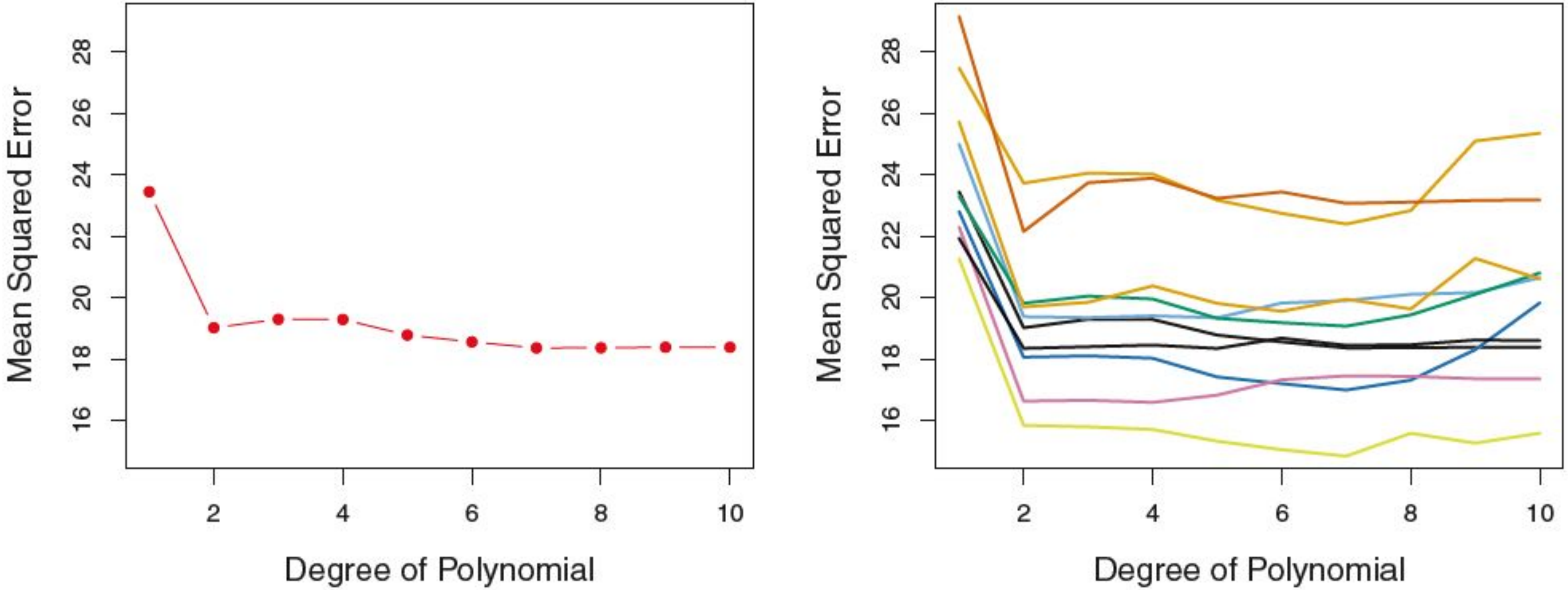
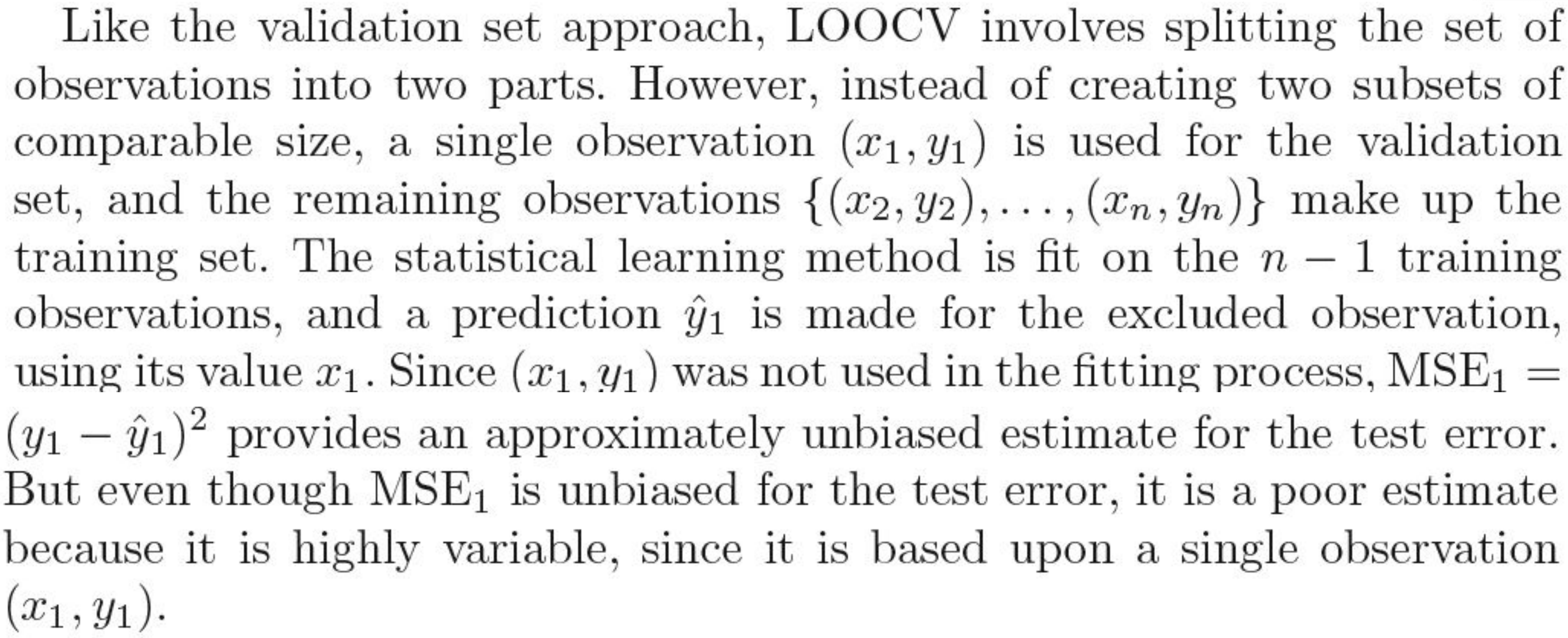


FIGURE 5.2. *The validation set approach was used on the* Auto *data set in order to estimate the test error that results from predicting* mpg *using polynomial functions of* horsepower. Left: *Validation error estimates for a single split into training and validation data sets.* Right: *The validation method was repeated ten times, each time using a different random split of the observations into a training set and a validation set. This illustrates the variability in the estimated test MSE that results from this approach.*

Potential drawbacks

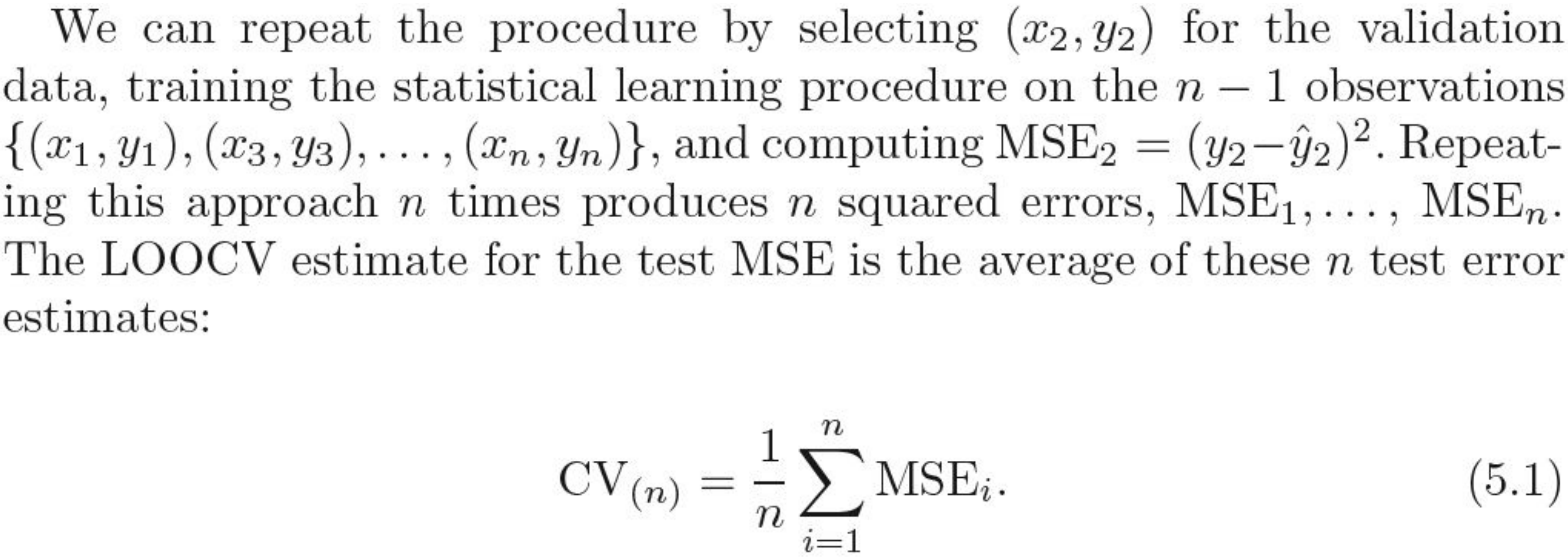
1. The validation estimate of the test error rate can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set.
2. In the validation approach, only a subset of the observations—those that are included in the training set rather than in the validation set—are used to fit the model. Since statistical methods tend to perform worse when trained on fewer observations, this suggests that the validation set error rate may tend to overestimate the test error rate for the model fit on the entire data set.

Leave-One-Out Cross-Validation (LOOCV)



Like the validation set approach, LOOCV involves splitting the set of observations into two parts. However, instead of creating two subsets of comparable size, a single observation (x_1, y_1) is used for the validation set, and the remaining observations $\{(x_2, y_2), \ldots, (x_n, y_n)\}$ make up the training set. The statistical learning method is fit on the $n - 1$ training observations, and a prediction $\hat{y}_1$ is made for the excluded observation, using its value x_1. Since (x_1, y_1) was not used in the fitting process, $\text{MSE}_1 = (y_1 - \hat{y}_1)^2$ provides an approximately unbiased estimate for the test error. But even though MSE_1 is unbiased for the test error, it is a poor estimate because it is highly variable, since it is based upon a single observation (x_1, y_1).

Leave-One-Out Cross-Validation (LOOCV)



We can repeat the procedure by selecting (x_2, y_2) for the validation data, training the statistical learning procedure on the $n-1$ observations $\{(x_1, y_1), (x_3, y_3), \ldots, (x_n, y_n)\}$, and computing $\text{MSE}_2 = (y_2 - \hat{y}_2)^2$. Repeating this approach n times produces n squared errors, $\text{MSE}_1, \ldots, \text{MSE}_n$. The LOOCV estimate for the test MSE is the average of these n test error estimates:

$$\text{CV}_{(n)} = \frac{1}{n} \sum_{i=1}^{n} \text{MSE}_i. \qquad (5.1)$$

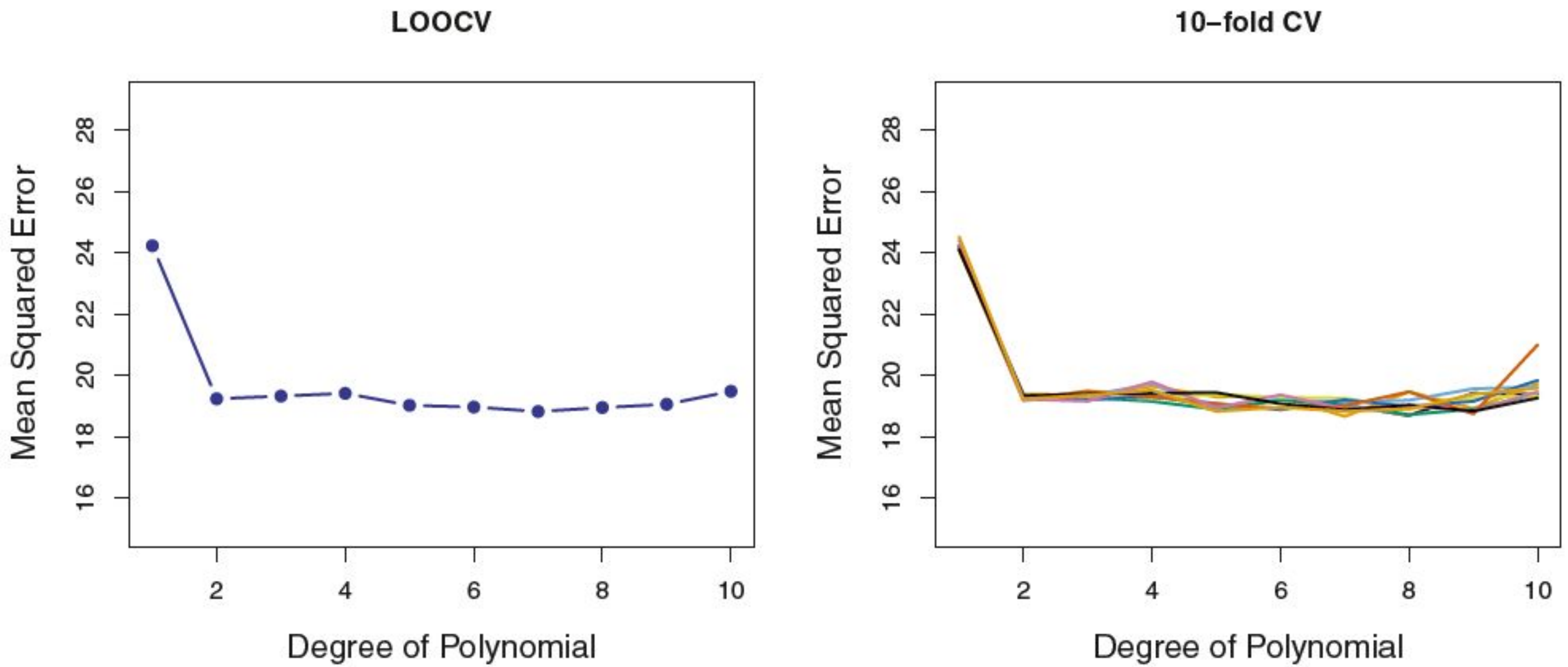
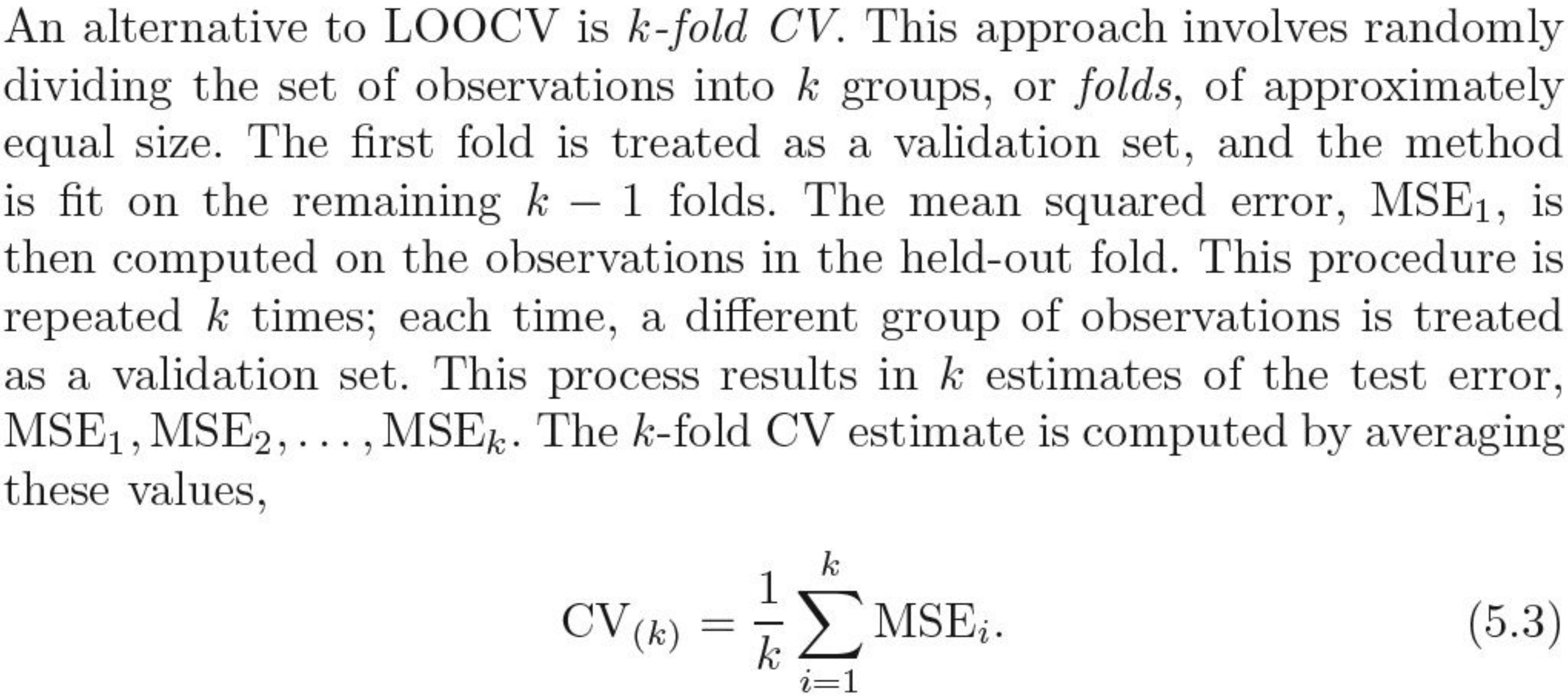


FIGURE 5.4. *Cross-validation was used on the* `Auto` *data set in order to estimate the test error that results from predicting* `mpg` *using polynomial functions of* `horsepower`. Left: *The LOOCV error curve.* Right: 10-*fold CV was run nine separate times, each with a different random split of the data into ten parts. The figure shows the nine slightly different CV error curves.*

Leave-One-Out Cross-Validation (LOOCV)

- Expensive to implement
- General method
- Can be used with any predictive model

k-Fold Cross-Validation



An alternative to LOOCV is *k-fold CV*. This approach involves randomly dividing the set of observations into k groups, or *folds*, of approximately equal size. The first fold is treated as a validation set, and the method is fit on the remaining $k - 1$ folds. The mean squared error, MSE_1, is then computed on the observations in the held-out fold. This procedure is repeated k times; each time, a different group of observations is treated as a validation set. This process results in k estimates of the test error, $\mathrm{MSE}_1, \mathrm{MSE}_2, \ldots, \mathrm{MSE}_k$. The k-fold CV estimate is computed by averaging these values,

$$\mathrm{CV}_{(k)} = \frac{1}{k}\sum_{i=1}^{k} \mathrm{MSE}_i. \tag{5.3}$$

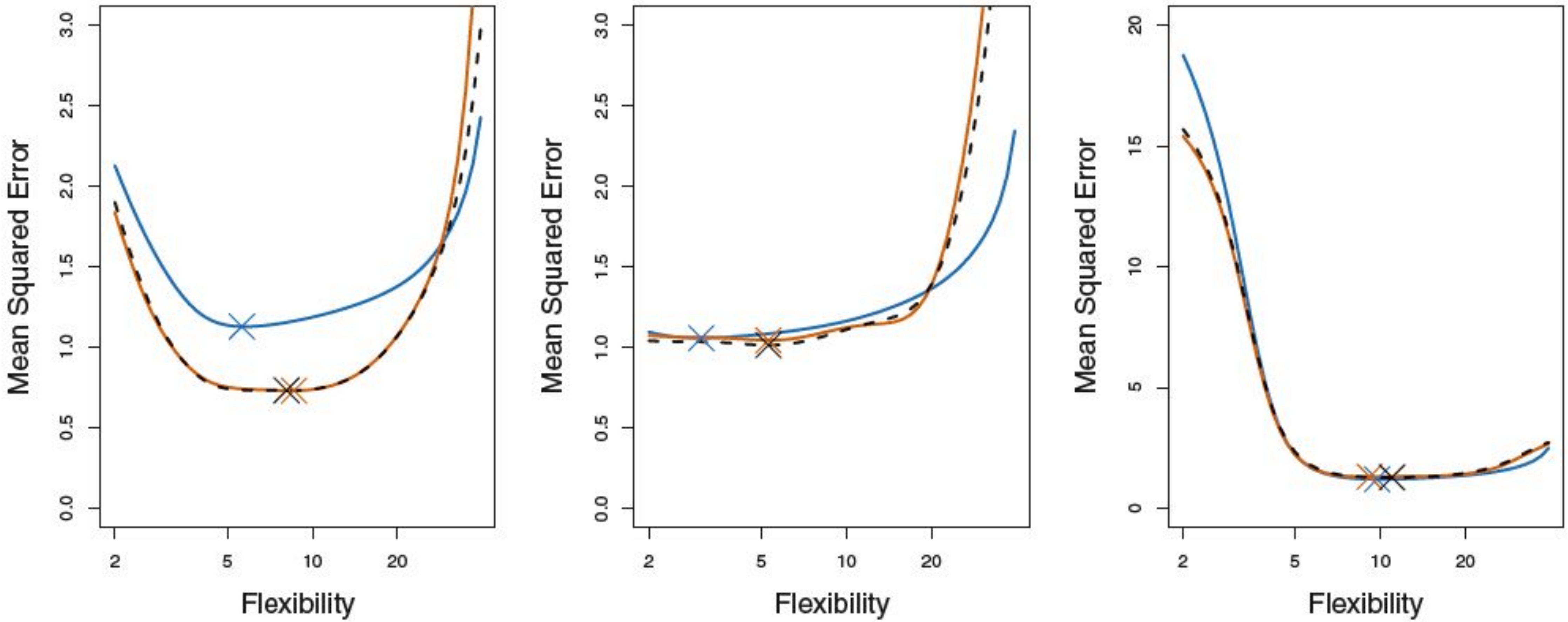
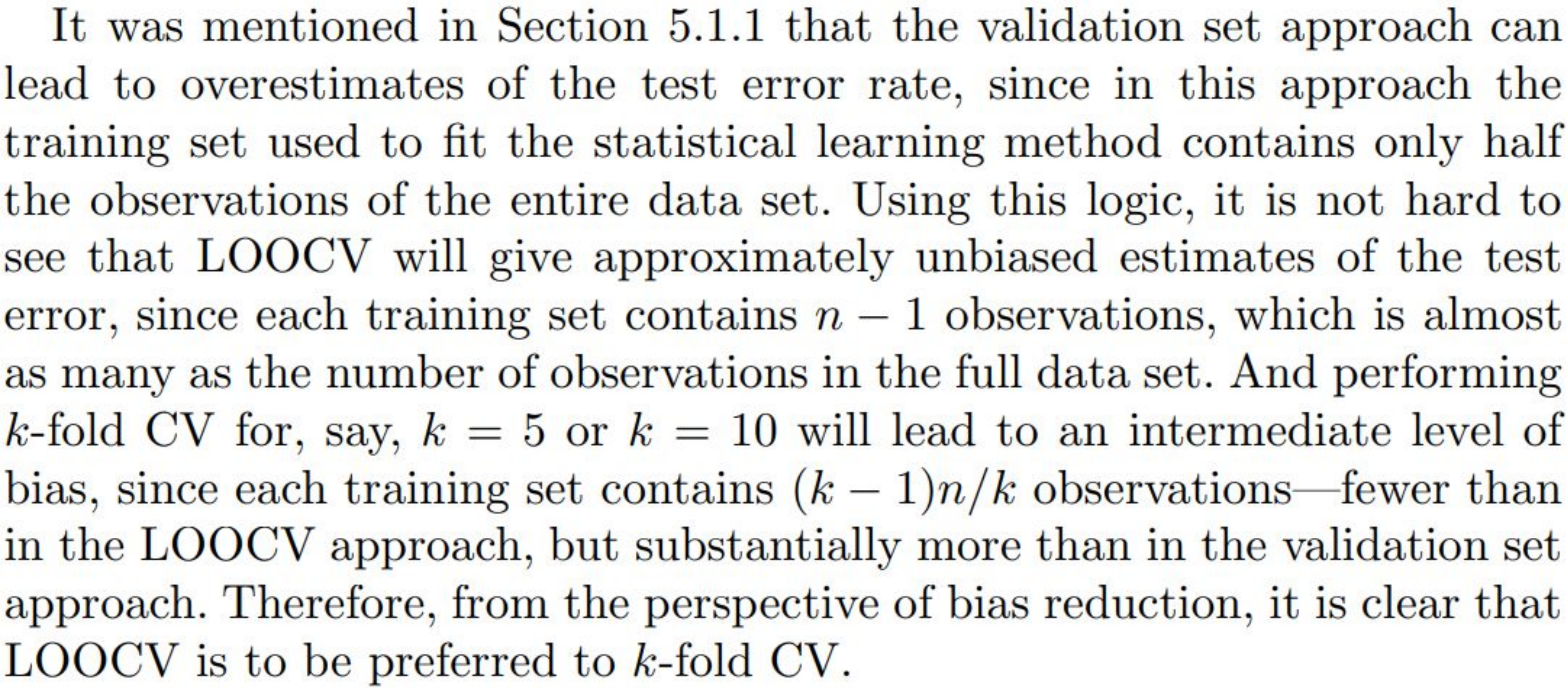


FIGURE 5.6. *True and estimated test MSE for the simulated data sets in Figures 2.9 (*left*), 2.10 (*center*), and 2.11 (*right*). The true test MSE is shown in blue, the LOOCV estimate is shown as a black dashed line, and the* 10*-fold CV estimate is shown in orange. The crosses indicate the minimum of each of the MSE curves.*

Bias-Variance Trade-Off for k-Fold Cross-Validation

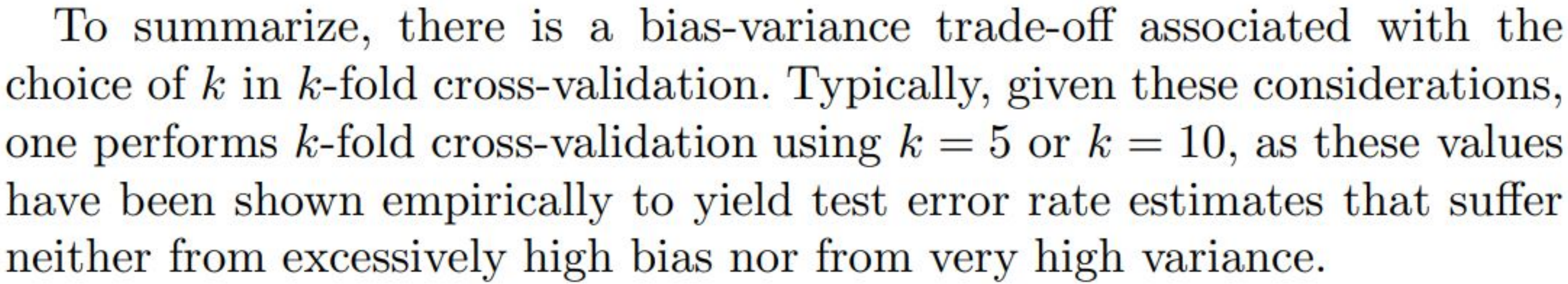
- Advantage of k-fold CV is that it often gives more accurate estimates of the test error rate than does LOOCV.
- This has to do with a bias-variance trade-off.



It was mentioned in Section 5.1.1 that the validation set approach can lead to overestimates of the test error rate, since in this approach the training set used to fit the statistical learning method contains only half the observations of the entire data set. Using this logic, it is not hard to see that LOOCV will give approximately unbiased estimates of the test error, since each training set contains $n-1$ observations, which is almost as many as the number of observations in the full data set. And performing k-fold CV for, say, $k = 5$ or $k = 10$ will lead to an intermediate level of bias, since each training set contains $(k-1)n/k$ observations—fewer than in the LOOCV approach, but substantially more than in the validation set approach. Therefore, from the perspective of bias reduction, it is clear that LOOCV is to be preferred to k-fold CV.

Bias-Variance Trade-Off for k-Fold Cross-Validation

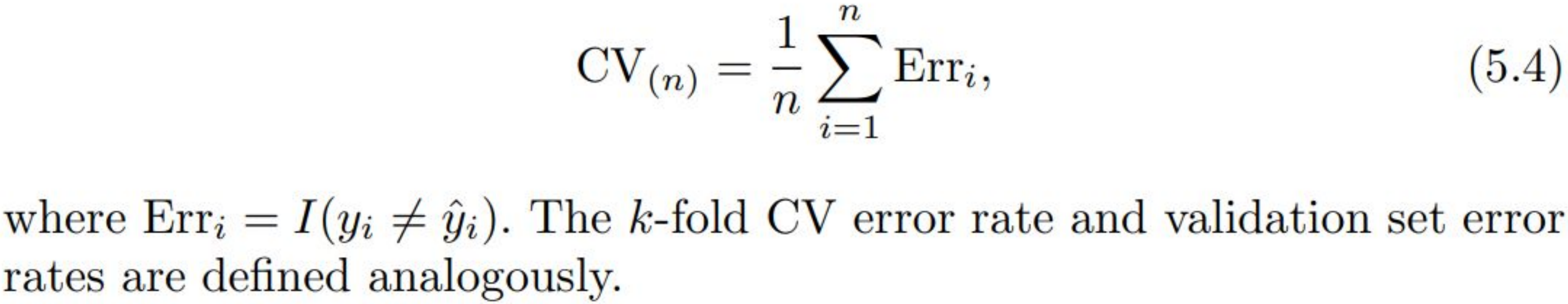
- It turns out that LOOCV has higher variance than does k-fold CV with k<n.
- When we perform LOOCV, we are in effect averaging the outputs of n fitted models, each of which is trained on an almost identical set of observations; therefore, these outputs are highly (positively) correlated with each other.
- In contrast, when we perform k-fold CV with k<n, we are averaging the outputs of k fitted models that are somewhat less correlated with each other, since the overlap between the training sets in each model is smaller.



To summarize, there is a bias-variance trade-off associated with the choice of k in k-fold cross-validation. Typically, given these considerations, one performs k-fold cross-validation using $k = 5$ or $k = 10$, as these values have been shown empirically to yield test error rate estimates that suffer neither from excessively high bias nor from very high variance.

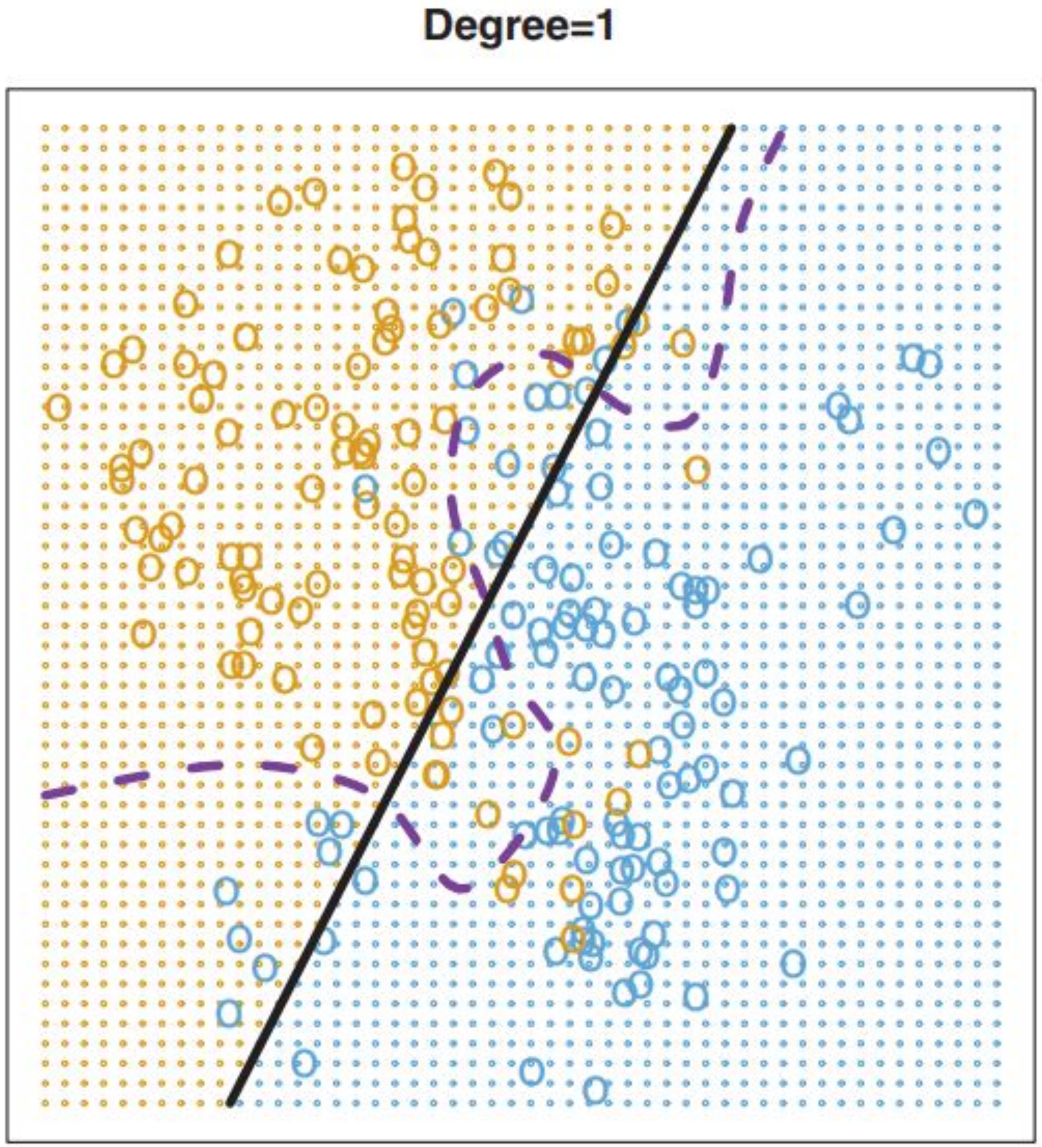
Cross-Validation on Classification Problems

In the classification setting, the LOOCV error rate takes the form

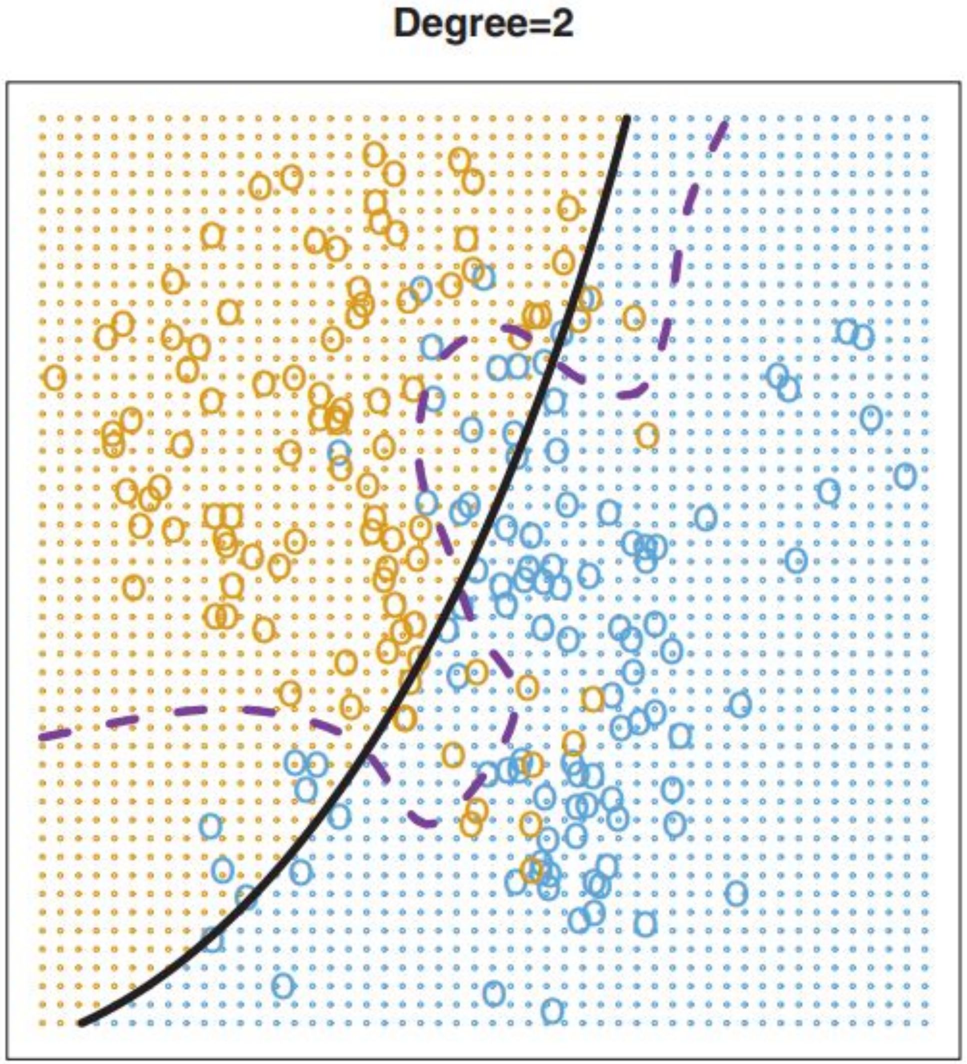


$$\mathrm{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n} \mathrm{Err}_i, \tag{5.4}$$

where $\mathrm{Err}_i = I(y_i \neq \hat{y}_i)$. The k-fold CV error rate and validation set error rates are defined analogously.



Logistic regression fits on the two-dimensional classification data. The Bayes decision boundary is represented using a purple dashed line. Estimated decision boundaries from linear, quadratic, cubic and quartic (degrees 1–4) logistic regressions are displayed in black. The test error rates for the four logistic regression fits are respectively 0.201, 0.197, 0.160, and 0.162, while the Bayes error rate is 0.133.



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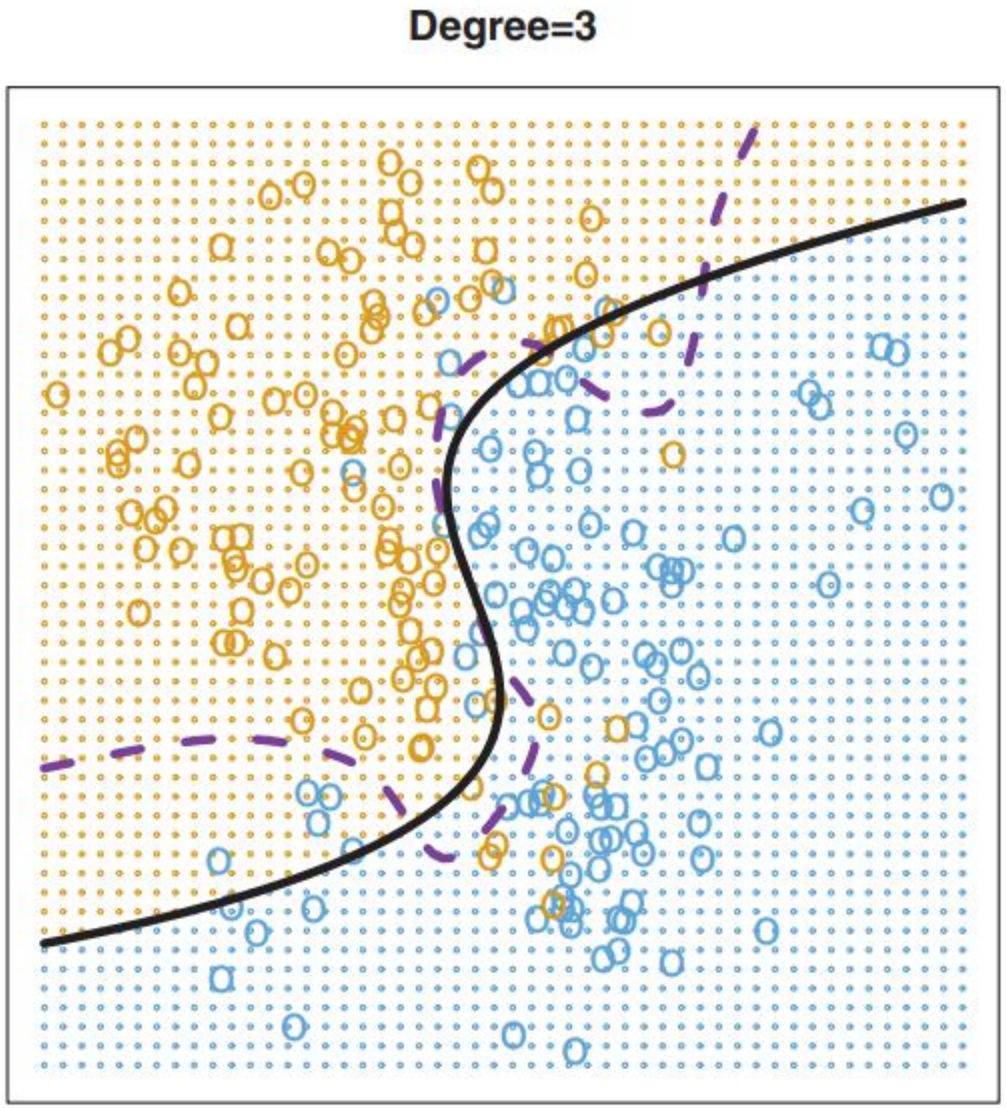

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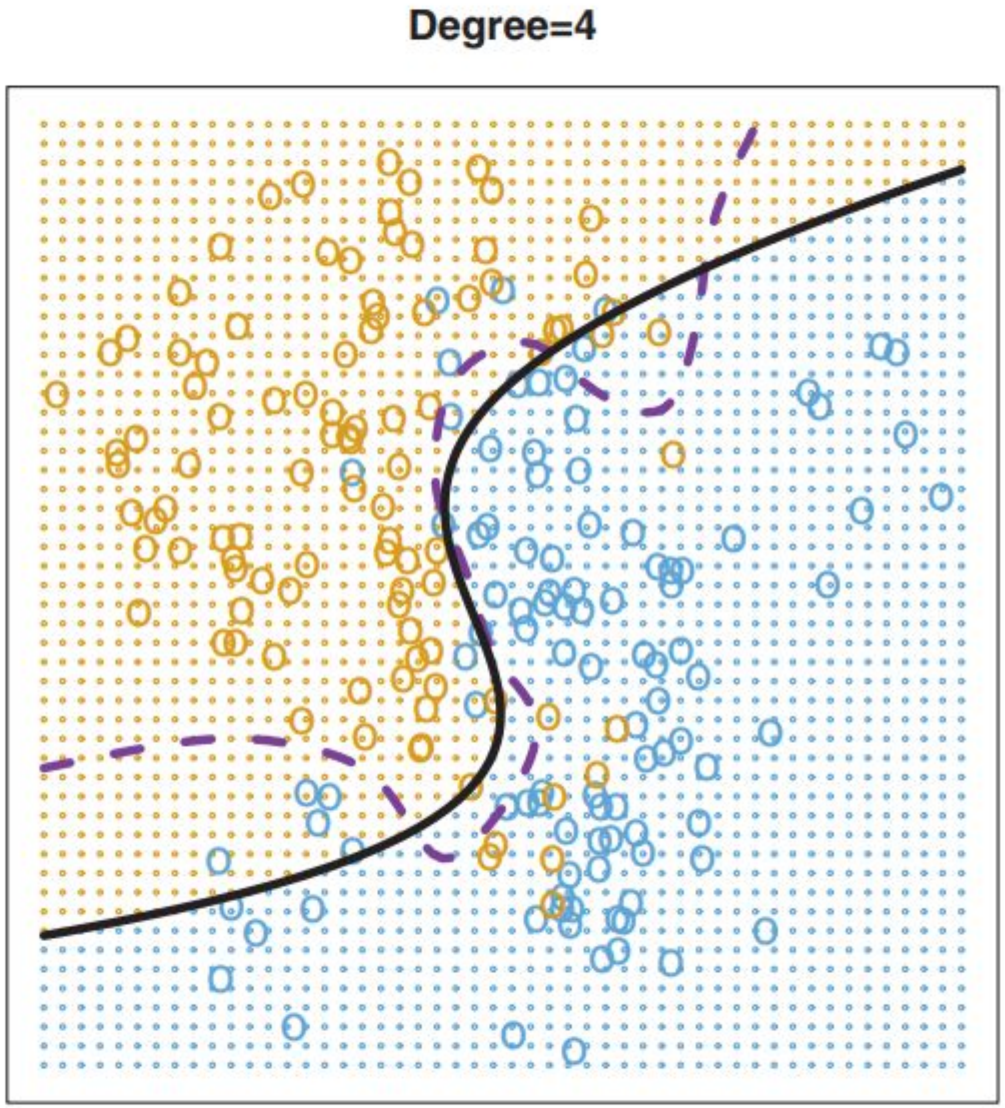

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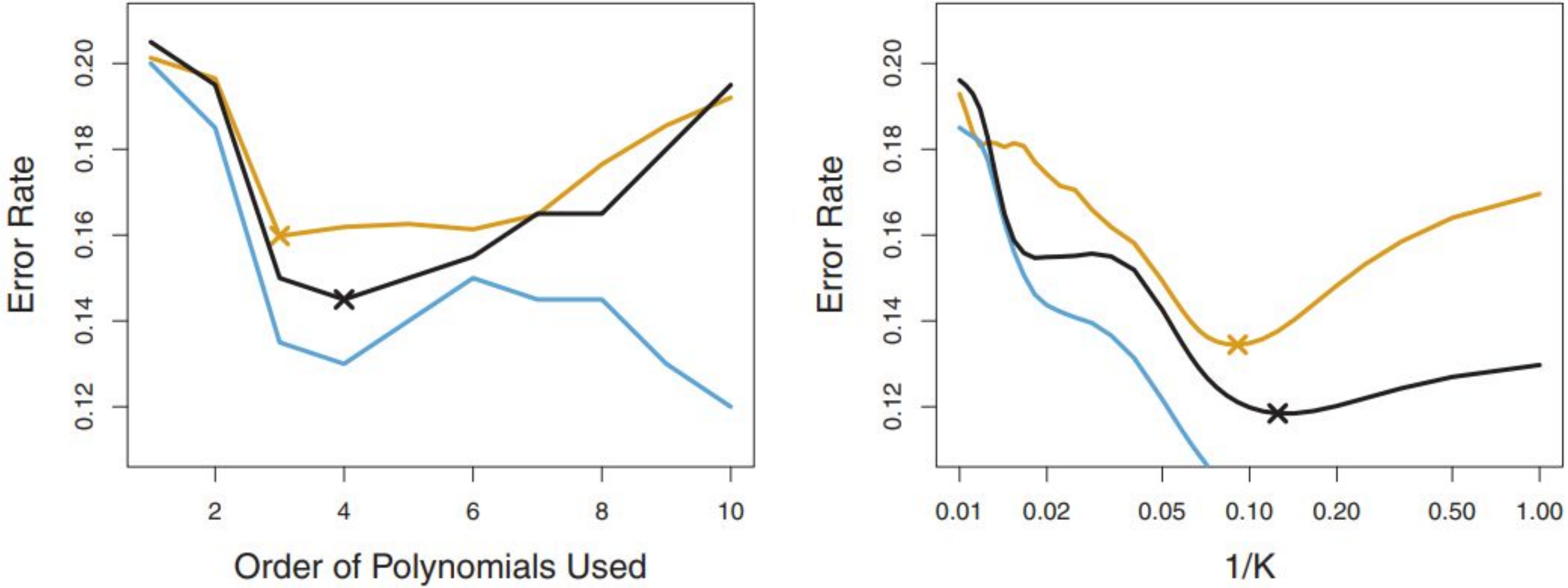

FIGURE 5.8. *Test error (brown), training error (blue), and* 10*-fold CV error (black) on the two-dimensional classification data displayed in Figure 5.7.* Left: *Logistic regression using polynomial functions of the predictors. The order of the polynomials used is displayed on the x-axis.* Right: *The KNN classifier with different values of K, the number of neighbors used in the KNN classifier.*

The Bootstrap

Assignment