01. Statistical Learning and Cross-validation

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Statistical Learning

- Statistical learning is a set of tools for modeling and understanding complex datasets.
- It is recently developed area in statistics along with machine learning in computer science.
- With the explosion of "Big Data" problems, statistical learning has become a very hot field in many scientific areas.
- The tools of statistical learning can be classified as supervised or unsupervised learning.
- Supervised statistical learning builds a statistical model for predicting or estimating for data with an output based on one or more inputs.
- Unsupervised statistical learning learns relationships and structure from data that has inputs but no supervising output.

Supervised Learning Problem

- Outcome measurement Y (also called dependent variable, response, target).
- Vector of p predictor measurements X (also called independent variables, inputs, regressors, features).
- In the regression problem, Y is quantitative (e.g numerical values such as blood pressure and weight).
- In the classification problem, Y takes values in a finite, unordered set (survived/died, cancer class of tissue sample, case/control).
- We have n observations consisting of $(x_1, y_1), \ldots, (x_n, y_n)$, where

$$x_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^{\mathrm{T}}$$

  is the p-dimensional vector.

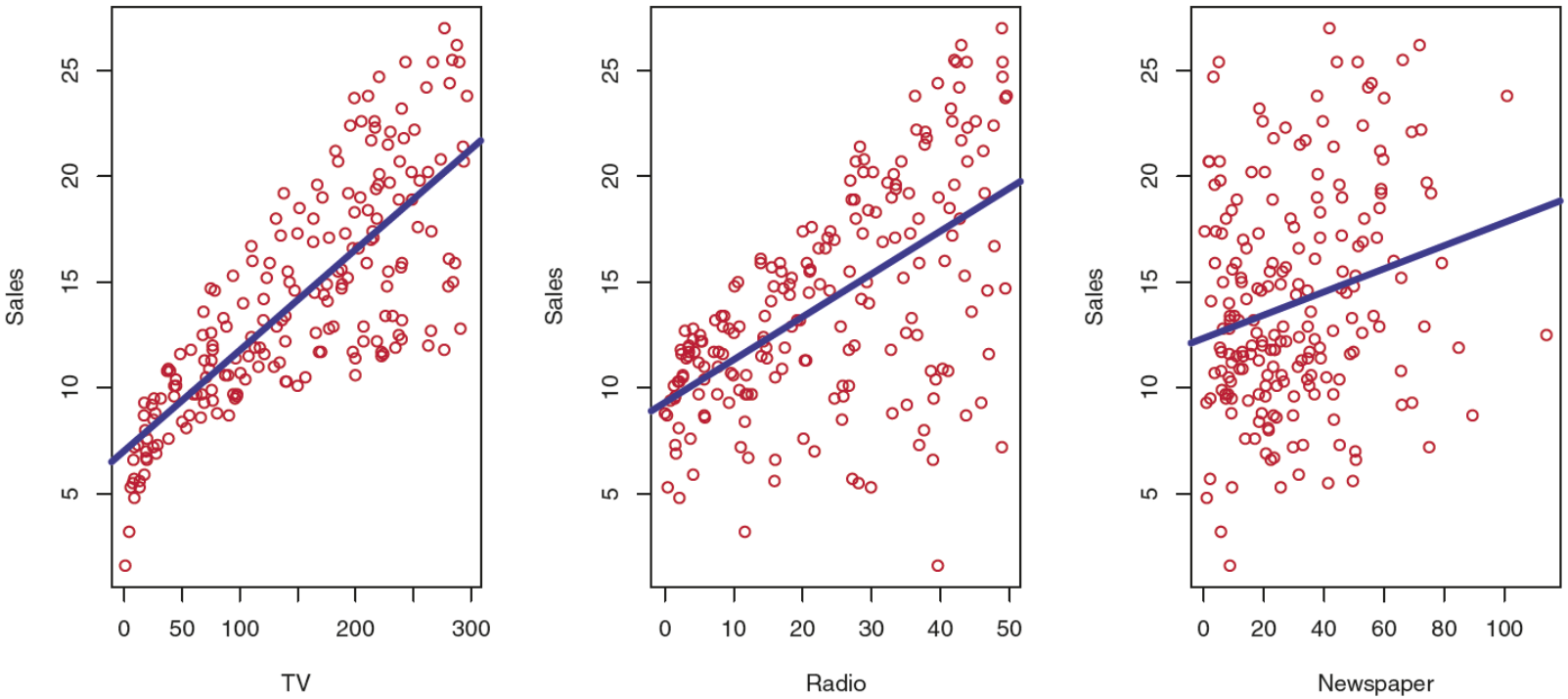
Objectives and Philosophy

- On the basis of the training data we would like to:
  - Accurately predict unseen test cases.
  - Understand which inputs affect the outcome, and how.
  - Assess the quality of our predictions and inferences.
- Philosophy
  - It is important to understand the ideas behind the various techniques, in order to know how and when to use them.
  - One has to understand the simpler methods first, in order to grasp the more sophisticated ones.
  - It is important to accurately assess the performance of a method, to know how well or how badly it is working (simpler methods often perform as well as fancier ones!)
  - This is an exciting research area, having important applications in high-dimensional data analysis.

Statistical Learning vs. Machine Learning

- Machine learning arose as a subfield of Artificial Intelligence.
- Statistical learning arose as a subfield of Statistics.
- There is much overlap – both fields focus on supervised and unsupervised problems:
  - Machine learning has a greater emphasis on large scale applications and prediction accuracy.
  - Statistical learning emphasizes models, interpretability, precision and uncertainty.
- But, the distinction has become more and more blurred, and there is a great deal of "cross-fertilization".

Advertising Data



- Shown are Sales vs TV, Radio and Newspaper, with a blue linear-regression line fit separately to each.
- Can we predict Sales using these three?
- Perhaps we can do better using a model

$$\text{Sales} \approx f(\text{TV, Radio, Newspaper})$$

Advertising Data

```
## Open the dataset linked to the book website
url.ad <- "https://www.statlearning.com/s/Advertising.csv"
Advertising <- read.csv(url.ad, h=T)
attach(Advertising)
```

```
## Least square fit for simple linear regression
par(mfrow = c(1,3))
plot(sales~TV, col=2, xlab="TV", ylab="Sales")
abline(lm(sales~TV)$coef, lwd=3, col="darkblue")
```

```
plot(sales~radio, col=2, xlab="Radio", ylab="Sales")
abline(lm(sales~radio)$coef, lwd=3, col="darkblue")
```

```
plot(sales~newspaper, col=2, xlab="Newspaper", ylab="Sales")
abline(lm(sales~newspaper)$coef, lwd=3, col="darkblue")
```

Notation

- Here Sales is a response or target that we wish to predict. We generically refer to the response as Y.
- TV is a feature, or input, or predictor; we name it X_1. Likewise name Radio as X_2, and so on.
- We can refer to the input vector collectively as

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix}$$

- We assume that there is some relationship between Y and $X = (X_1, X_2, X_3)^{\mathrm{T}}$

Supervised Learning: Model

- Now we write our model as

$$Y = f(X) + \epsilon$$

  where ϵ captures measurement errors and other discrepancies.
- With a good $f(\cdot)$ we can make predictions of Y at new points $X = x$.
- Depending on the complexity of $f(\cdot)$, we may be able to understand how each component X_j of X affects Y.
- The function f that connects the input variable to the output variable is in general unknown.
- Statistical learning refers to a set of approaches for estimating the function f.

Advertising Data

```
AD <- Advertising[ ,-1]
```

```
## Multiple linear regression
lm.fit <- lm(sales ~., AD)
summary(lm.fit)
names(lm.fit)
coef(lm.fit)
confint(lm.fit)
```

```
par(mfrow=c(2,2))
plot(lm.fit)
```

```
dev.off()
plot(predict(lm.fit), residuals(lm.fit))
plot(predict(lm.fit), rstudent(lm.fit))
plot(hatvalues(lm.fit))
which.max(hatvalues(lm.fit))
```

Estimation of f for Prediction

- There are two main reasons that we may wish to estimate f:
  - prediction
  - inference
- We can predict

$$\hat{Y} = \hat{f}(X)$$

  where $\hat{f}$ represents our estimate for f, and $\hat{Y}$ represents the resulting prediction for Y.
- In this setting, $\hat{f}$ is often treated as a black box, in the sense that one is not typically concerned with the exact form of $\hat{f}$, provided that it yields accurate predictions for Y.
- Statistically, ideal function $f(\cdot)$ is

$$f(x) = E(Y|X = x)$$

  which is called the regression function.

How to find $f(\cdot)$

- For any estimate $\hat{f}(x)$ of $f(x)$, we have

$$E[(Y - \hat{f}(X))^2 | X = x] = E[f(x) + \epsilon - \hat{f}(x)]^2$$
$$= \underbrace{E[(f(x) - \hat{f}(x)]^2}_{\text{Reducible}} + \underbrace{Var(\epsilon)}_{\text{Irreducible}}$$

- Irreducible error: even if we knew $f(x)$, we would still make errors in prediction, since at each $X = x$ there is typically a distribution of possible Y values.

$$\epsilon = Y - f(x)$$

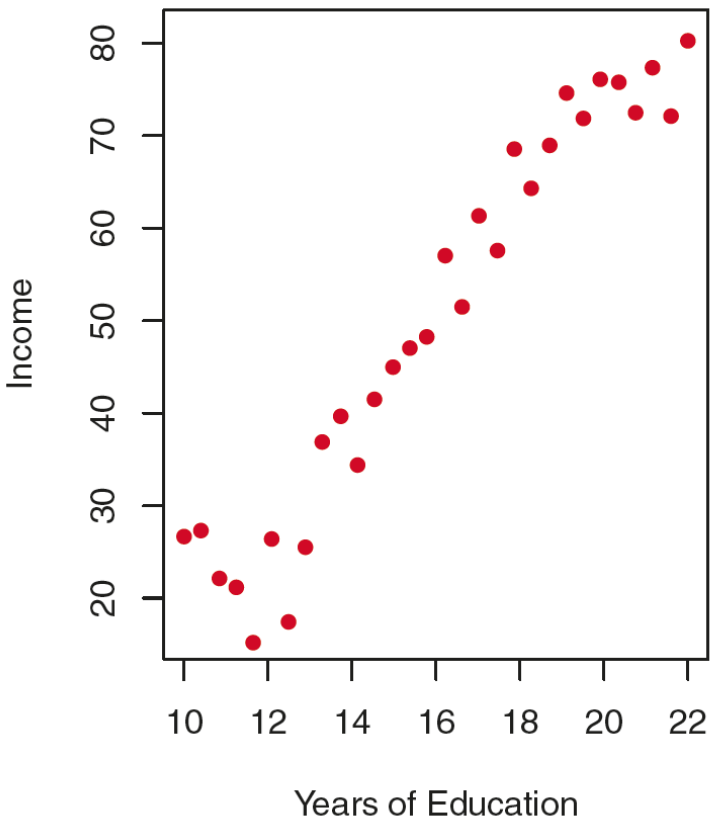
- The focus is on statistical learning techniques for estimating f with the aim of minimizing the reducible error.

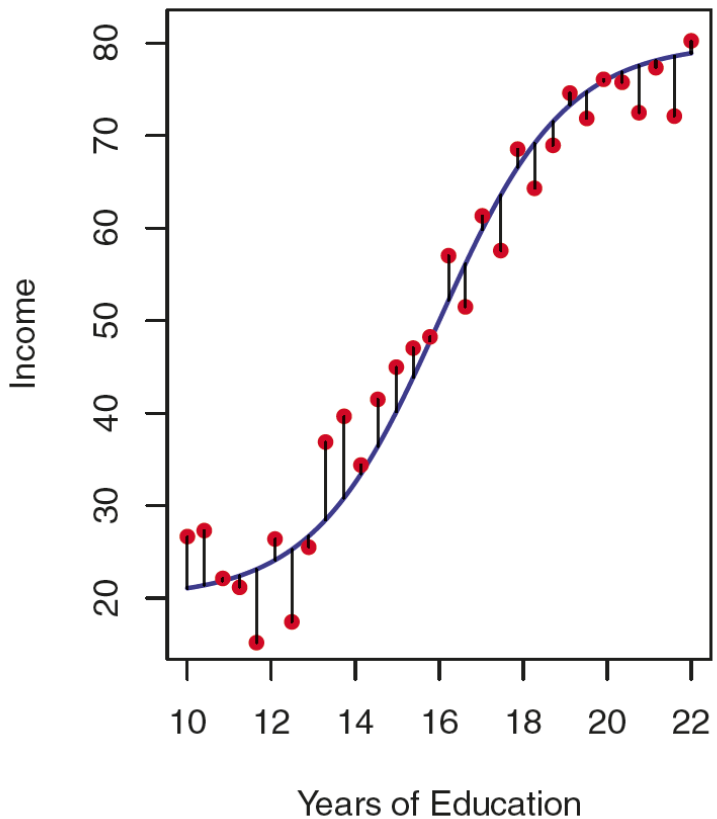
Estimation of f for Inference

- We are often interested in understanding the way that Y is affected as $X_1, \ldots, X_p$ change.
- In this situation we wish to estimate f, but our goal is not necessarily to make predictions for Y.
- Now $\hat{f}$ cannot be treated as a black box, because we need to know its exact form.
- In this setting, one may be interested in answering the following questions:
  - Which predictors are associated with the response?
  - What is the relationship between the response and each predictor?
  - Can the relationship between Y and each predictor be adequately summarized using a linear equation, or is the relationship more complicated?

Income Data

- As another example, a plot of income versus years of education for 30 individuals in the Income data set.
- The plot suggests that one might be able to predict income using years of education.





Income Data

```
url.in <- "https://www.statlearning.com/s/Income1.csv"
Income <- read.csv(url.in, h=T)
```

```
## Polynomial regression fit
par(mfrow = c(1,2))
plot(Income~Education, col=2, pch=19, xlab="Years of Education",
     ylab="Income", data=Income)
g <- lm(Income ~ poly(Education, 3), data=Income)
```

```
plot(Income~Education, col=2, pch=19, xlab="Years of Education",
     ylab="Income", data=Income)
lines(Income$Education, g$fit, col="darkblue", lwd=4,
      ylab="Income", xlab="Years of Education")
```

```
y <- Income$Income
mean((predict(g) - y)^2)
mean(residuals(g)^2)
```

Income Data

```
dist <- NULL
```

```
par(mfrow=c(3,4))
for (k in 1:12) {
   g <- lm(Income ~ poly(Education, k), data=Income)
   dist[k] <- mean(residuals(g)^2)
   plot(Income~Education, col=2, pch=19,
        xlab="Years of Education", ylab="Income",
        data=Income, main=paste("k =", k))
   lines(Income$Education,g$fit,col="darkblue",lwd=3,
         ylab="Income", xlab="Years of Education")
}
```

```
x11()
plot(dist, type="b", xlab="Degree of Polynomial",
     ylab="Mean squared distance")
```

Parametric and Non-parametric Methods

- Observations we have are called the training data because we use these observations to train or teach our method.
- Our goal is to apply a statistical learning method to the training data in order to estimate the unknown function f such that

$$Y \approx \hat{f}(X)$$

  for any observation (X, Y).
- Most statistical learning methods for this task can be characterized as either parametric or non-parametric.
  - Parametric methods: make an assumption about the functional form or shape of f.
  - Non-parametric methods: do not make explicit assumptions about the functional form of f.

Parametric Methods

- For example, f is assumed to be linear so,

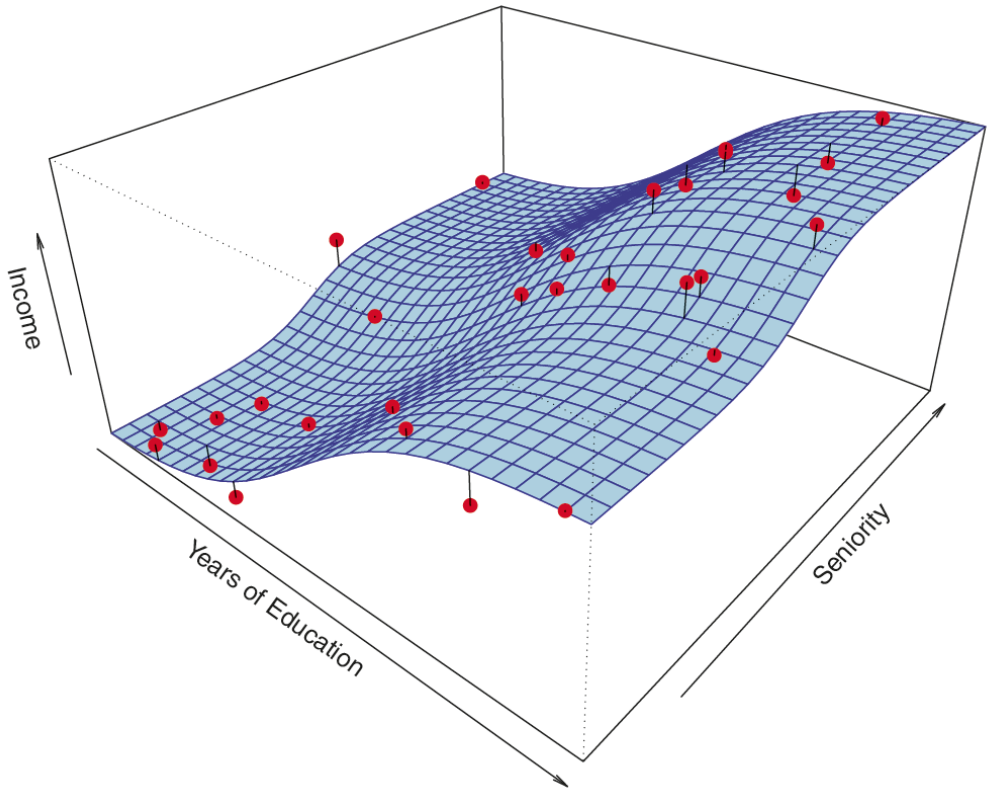
$$f(X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots, + \beta_p X_p + \epsilon,$$

  where we only needs to estimate $p + 1$ coefficients.
- Parametric methods reduce the problem of estimating f down to one of estimating a set of parameters.
- The disadvantage is that the model we choose will usually not match the true unknown form of f.
- If the chosen model is too far from the true f, then our estimate will be poor.
- Flexible models can fit many different possible functional forms for $f \rightarrow$ overfitting problem.

Non-parametric Methods

- Non-parametric methods estimates f that gets as close to data points as possible without being too rough or wiggly.
- They have the potential to accurately fit a wider range of possible shapes for f since they do not assume a particular functional form for f.
- No assumption about the form of f is made, so there is no danger that estimate f is very different from the true f.
- Since the number of parameters is not small, a very large number of observations is required in order to obtain an accurate estimate for f.
- There are advantages and disadvantages to parametric and non-parametric methods for statistical learning.

Example

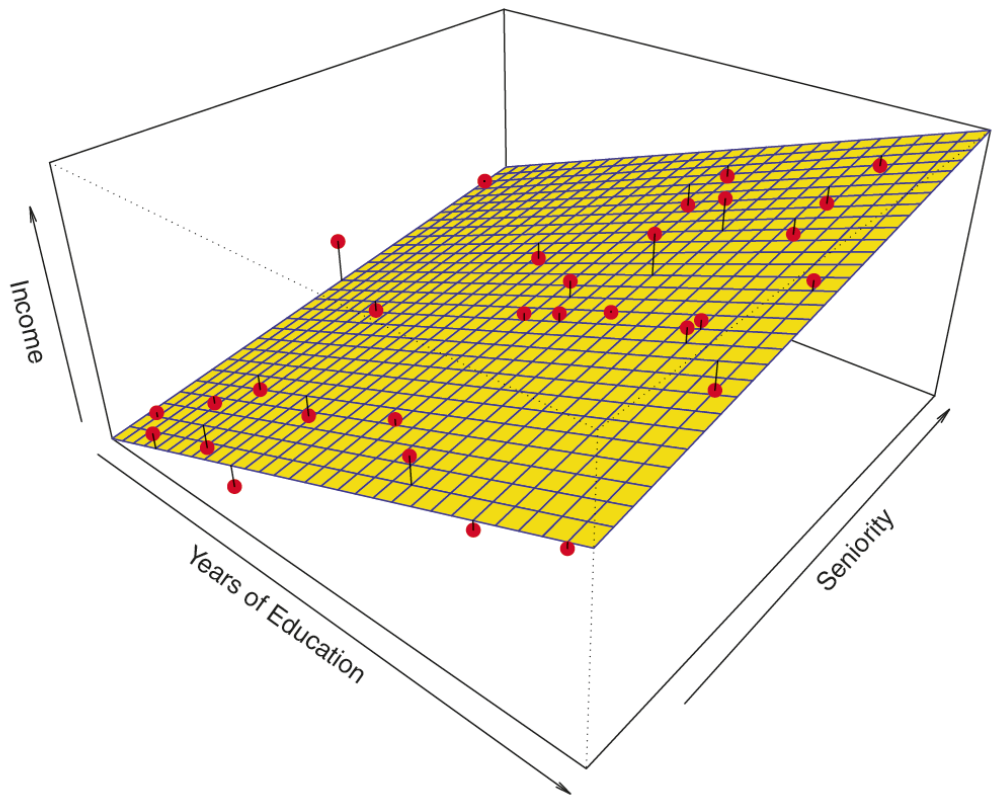


- Red points are simulated values for income from the model

$$\text{income} = f(\text{education, seniority}) + \epsilon$$

f is the blue surface.

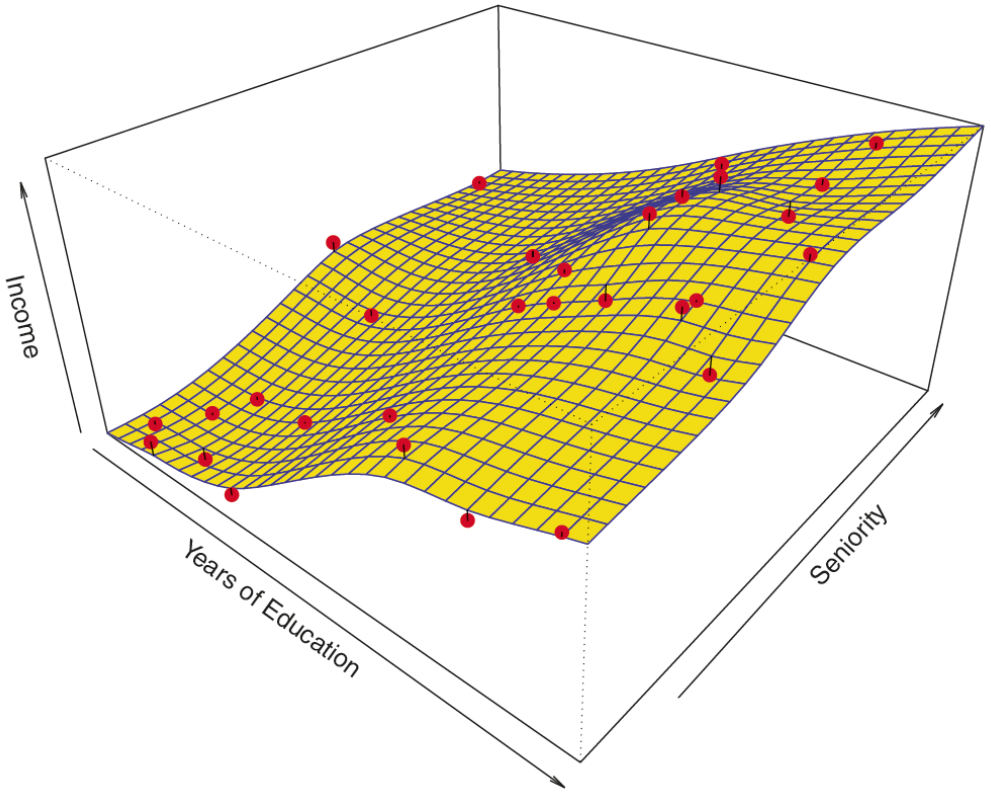
Linear Regression



- Linear regression model fit to the simulated data.

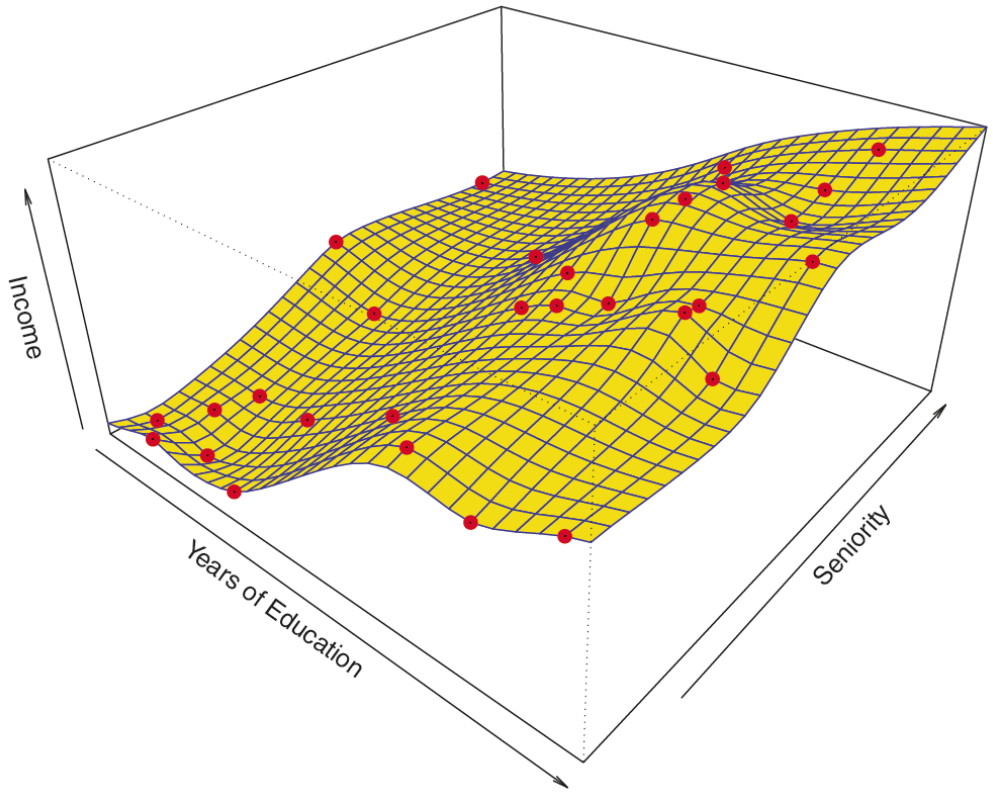
$$\hat{f}^L(\text{education, seniority}) = \hat{\beta}_0 + \hat{\beta}_1 \times \text{education} + \hat{\beta}_2 \times \text{seniority}$$

Thin-plate Spline



- More flexible regression model $\hat{f}^S(\text{education, seniority})$ fit to the simulated data.
- Here we use a technique called a thin-plate spline to fit a flexible surface.
- We can control the roughness of the fit.

Overfitting Spline



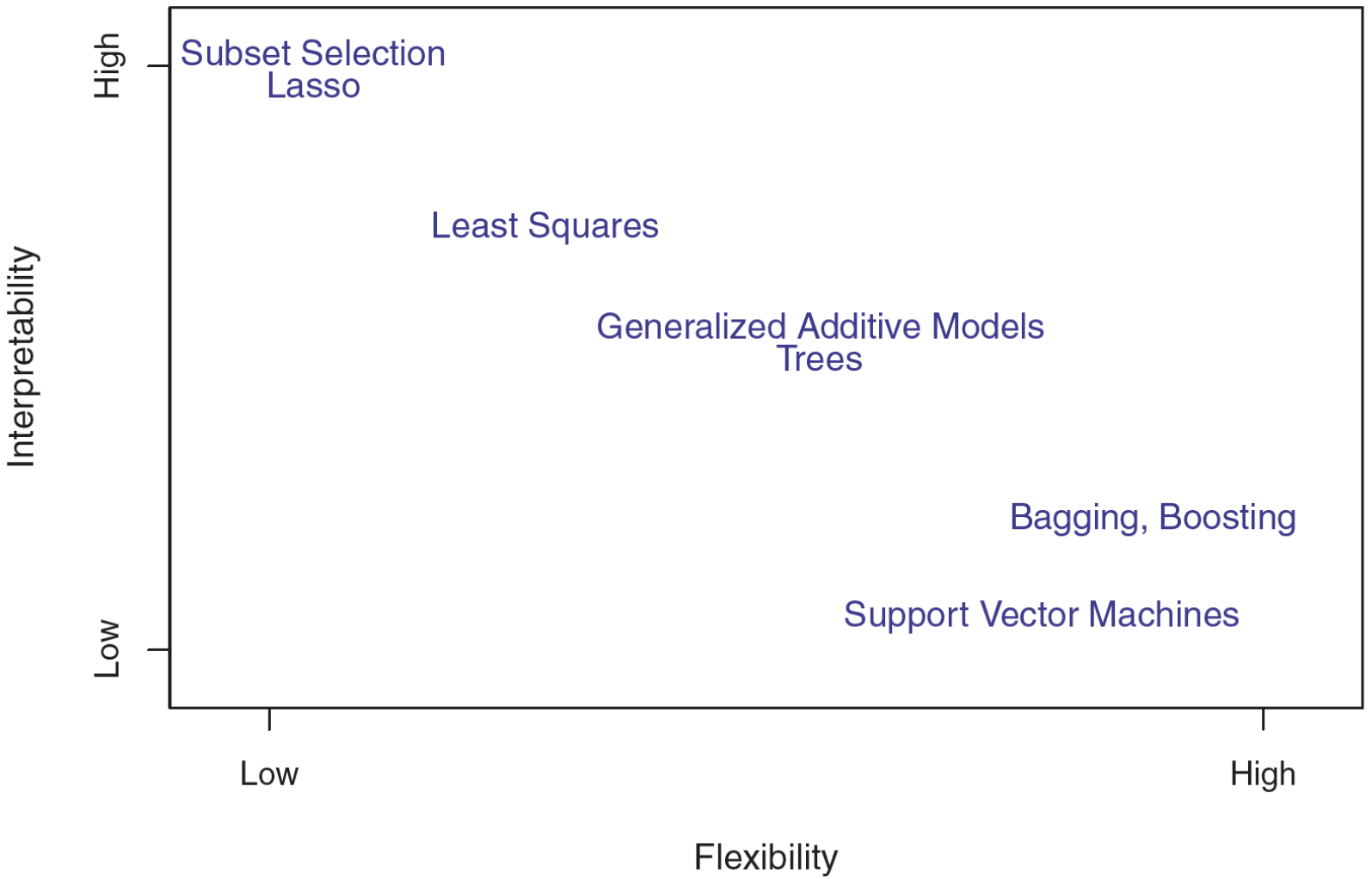
- Even more flexible spline regression model $\hat{f}^S(\text{education, seniority})$ fit to the simulated data.
- Here the fitted model makes no errors on the training data!
- This is known as a overfitting problem.

Flexibility and Interpretability

- Among many statistical learning methods, some are less flexible, or more restrictive.
- Linear regression is a relatively inflexible approach, because it can only generate linear functions.
- Thin plate splines are more flexible because they can generate a wider range of possible shapes to estimate f.
- If we are mainly interested in inference, then restrictive models are much more interpretable.
- Flexible approaches are difficult to understand how any individual predictor is associated with the response.
- If we are only interested in prediction, the most flexible model is preferable – often we can obtain more accurate predictions using a less flexible method.

Flexibility and Interpretability

- Trade-off between flexibility and interpretability.



Assessing Model Accuracy

- Why is it necessary to study so many different statistical learning approaches, rather than just a single best method?
- No one method dominates all others over all possible data sets

"*There is no free lunch in statistics*."

- On a particular data set, one specific method may work best, but some other method may work better on a similar but different data set.
- It is an important task to decide for any given set of data which method produces the best results.
- Selecting the best approach can be one of the most challenging parts of performing statistical learning in practice.

Assessing Model Accuracy

- In order to evaluate the performance of a statistical learning method, we need some way to measure how well its predictions actually match the observed data.
  - Quantitative response: mean squared error (MSE), ...
  - Qualitative response: classification error rate, ...
- Type of data sets
  - Training set: to fit statistical learning models
  - Validation set: to select the optimal tuning parameter
  - Test set: to select the best model
- We are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen test data.

Assessing Model Accuracy

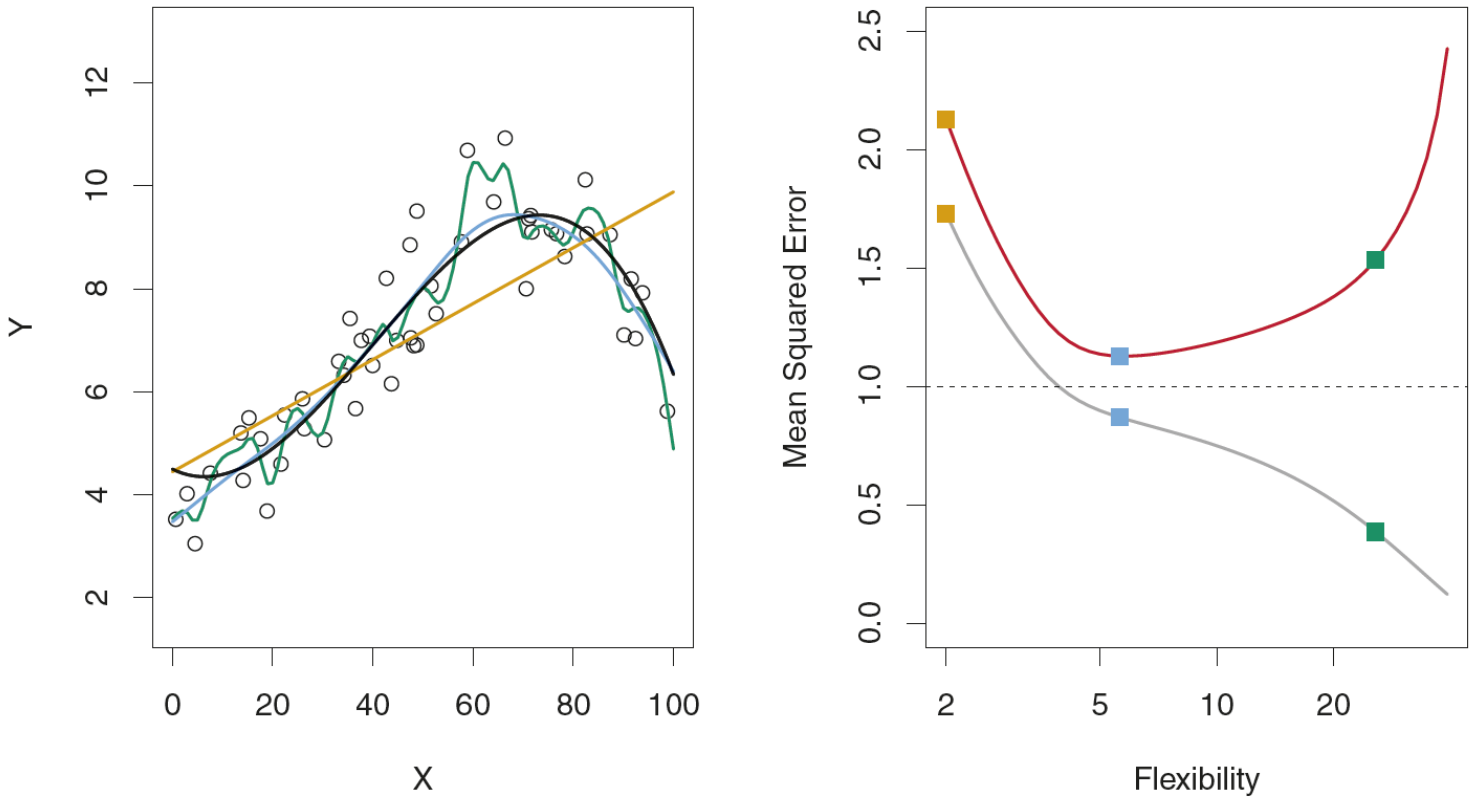
- Suppose we fit a model $\hat{f}(x)$ to some training data tran $= \{x_i, y_i\}_{i \in \{1,\ldots,n_1\}}$, and we see how well it performs.
- We could compute the average squared prediction error over training data:

$$MSE_{\text{tran}} = \frac{1}{n_1} \sum_{i \in \text{tran}} \left[y_i - \hat{f}(x_i) \right]^2$$

  This may be biased toward more overfit models.
- Instead we should, if possible, compute it using fresh test data test $= \{x_i, y_i\}_{i \in \{1,\ldots,n_2\}}$:

$$MSE_{\text{test}} = \frac{1}{n_2} \sum_{i \in \text{test}} \left[y_i - \hat{f}(x_i) \right]^2$$

Simulation Example: Cubic Model



- In the left, black curve is truth. Orange, blue and green curves/squares correspond to fits of different flexibility.
- Red curve on right is MSE_{test}, grey curve is MSE_{tran}.

Cubic Model

```
set.seed(12345)
```

```
## Simulate x and y based on a known function
fun1 <- function(x) -(x-100)*(x-30)*(x+15)/13^4+6
x <- runif(50,0,100)
y <- fun1(x) + rnorm(50)
```

```
## Plot linear regression and splines
par(mfrow=c(1,2))
plot(x, y, xlab="X", ylab="Y", ylim=c(1,13))
```

```
plot(x, y, xlab="X", ylab="Y", ylim=c(1,13))
lines(sort(x), fun1(sort(x)), col=1, lwd=2)
abline(lm(y~x)$coef, col="orange", lwd=2)
lines(smooth.spline(x,y, df=5), col="blue", lwd=2)
lines(smooth.spline(x,y, df=23), col="green", lwd=2)
legend("topleft", lty=1, col=c(1, "orange", "blue", "green"),
       legend=c("True", "df = 1", "df = 5", "df =23"),lwd=2)
```

Cubic Model

```
set.seed(45678)
```

```
## Simulate training and test data (x, y)
tran.x <- runif(50,0,100)
test.x <- runif(50,0,100)
tran.y <- fun1(tran.x) + rnorm(50)
test.y <- fun1(test.x) + rnorm(50)
```

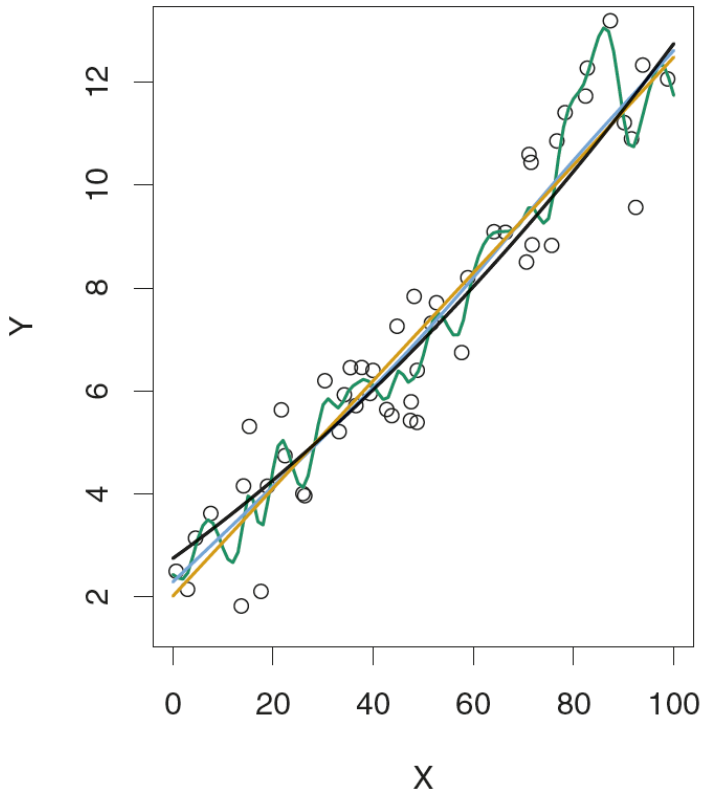
```
## Compute MSE along with different df
df <- 2:40
MSE <- matrix(0, length(df), 2)
for (i in 1:length(df)) {
    tran.fit <- smooth.spline(tran.x, tran.y, df=df[i])
    MSE[i,1] <- mean((tran.y - predict(tran.fit, tran.x)$y)^2)
    MSE[i,2] <- mean((test.y - predict(tran.fit, test.x)$y)^2)
}
```

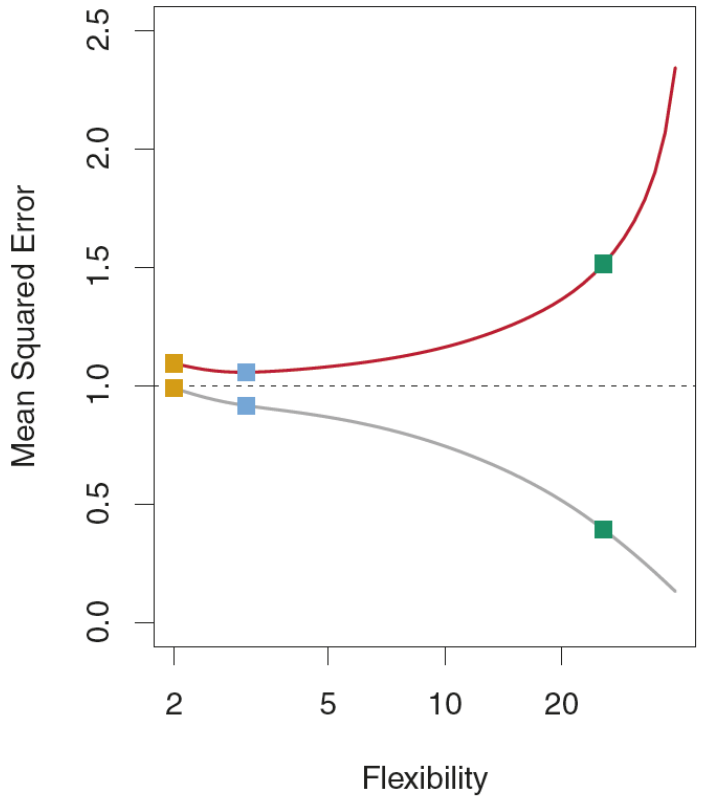
Cubic Model

```
## Plot both test and training errors
matplot(df, MSE, type="l", col=c("gray", "red"),
        xlab="Flexibility", ylab="Mean Squared Error",
        lwd=2, lty=1, ylim=c(0,4))
abline(h=1, lty=2)
legend("top", lty=1, col=c("red", "gray"),lwd=2,
       legend=c("Test MSE", "Training MSE"))
abline(v=df[which.min(MSE[,1])], lty=3, col="gray")
abline(v=df[which.min(MSE[,2])], lty=3, col="red")
```

```
matplot(df, MSE, type="l", col=c("gray", "red"),
        xlab="Flexibility", ylab="Mean Squared Error",
        lwd=2, lty=1, ylim=c(0.5,2), xlim=c(1,10))
abline(h=1, lty=2)
abline(v=df[which.min(MSE[,2])], lty=3, col="red")
```

Simulation Example: Linear Model





- Here the truth is a smoother, so the smoother fit and linear model do really well.

Linear Model

```
set.seed(12345)
```

```
## Simulate x and y based on a known function
fun2 <- function(x) x/10 +2
x <- runif(50,0,100)
y <- fun2(x) + rnorm(50)
```

```
## Plot linear regression and splines
par(mfrow=c(1,2))
plot(x, y, xlab="X", ylab="Y", ylim=c(1,13))
```

```
plot(x, y, xlab="X", ylab="Y", ylim=c(1,13))
lines(sort(x), fun2(sort(x)), col=1, lwd=2)
abline(lm(y~x)$coef, col="orange", lwd=2)
lines(smooth.spline(x,y, df=5), col="blue", lwd=2)
lines(smooth.spline(x,y, df=23), col="green", lwd=2)
legend("topleft", lty=1, col=c(1, "orange", "blue", "green"),
       legend=c("True", "df = 1", "df = 5", "df =23"),lwd=2)
```

Linear Model

```
set.seed(45678)
```

```
## Simulate training and test data (x, y)
tran.x <- runif(50,0,100)
test.x <- runif(50,0,100)
tran.y <- fun2(tran.x) + rnorm(50)
test.y <- fun2(test.x) + rnorm(50)
```

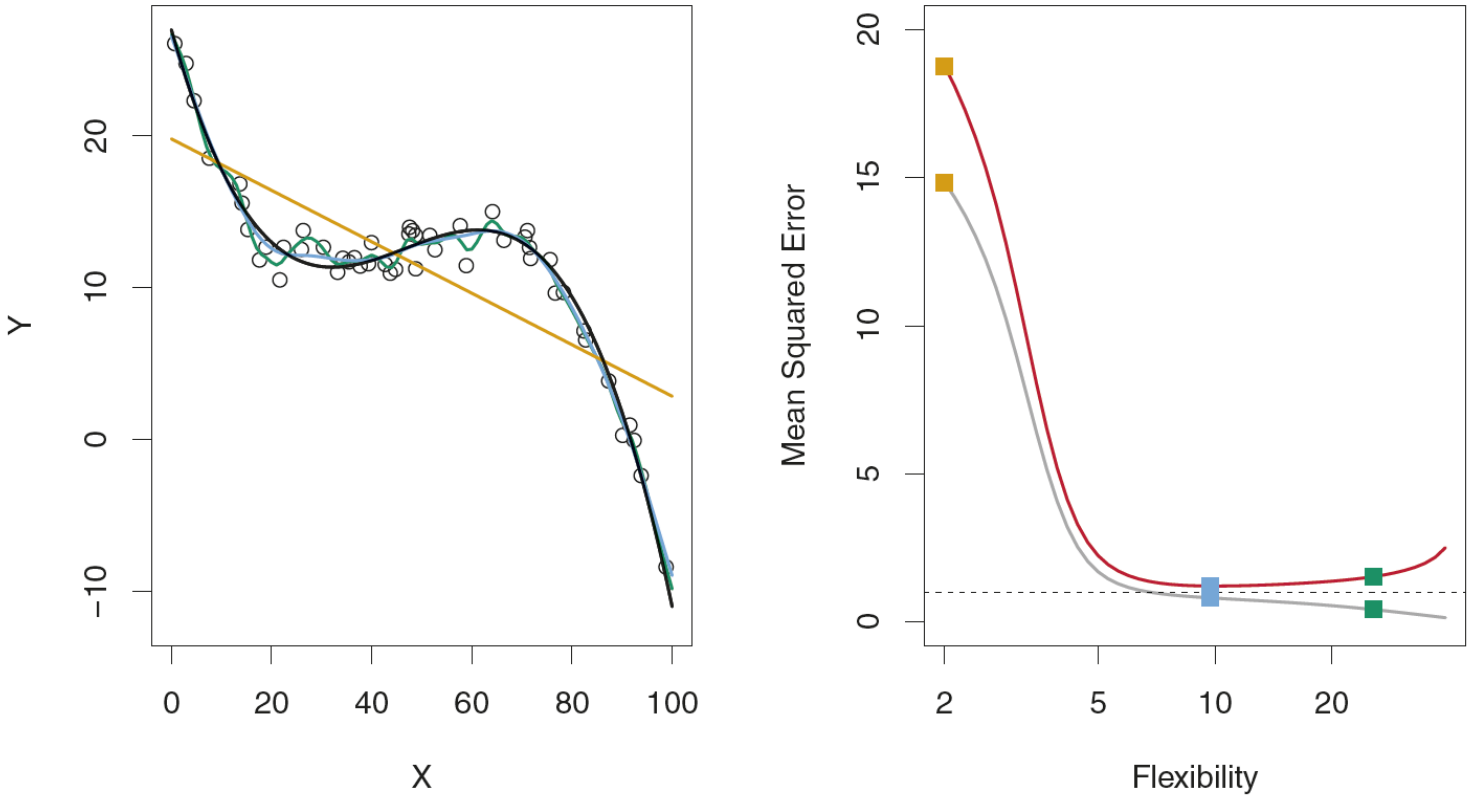
```
## Compute MSE along with different df
df <- 2:40
MSE <- matrix(0, length(df), 2)
for (i in 1:length(df)) {
    tran.fit <- smooth.spline(tran.x, tran.y, df=df[i])
    MSE[i,1] <- mean((tran.y - predict(tran.fit, tran.x)$y)^2)
    MSE[i,2] <- mean((test.y - predict(tran.fit, test.x)$y)^2)
}
```

Linear Model

```
## Plot both test and training errors
matplot(df, MSE, type="l", col=c("gray", "red"),
        xlab="Flexibility", ylab="Mean Squared Error",
        lwd=2, lty=1)
abline(h=1, lty=2)
legend("top", lty=1, col=c("red", "gray"),lwd=2,
       legend=c("Test MSE", "Training MSE"))
abline(v=df[which.min(MSE[,1])], lty=3, col="gray")
abline(v=df[which.min(MSE[,2])], lty=3, col="red")
```

```
matplot(df, MSE, type="l", col=c("gray", "red"),
        xlab="Flexibility", ylab="Mean Squared Error",
        lwd=2, lty=1, ylim=c(0,1.5), xlim=c(1,10))
abline(h=1, lty=2)
abline(v=df[which.min(MSE[,2])], lty=3, col="red")
```

Simulation Example: Nonlinear Model



- Here the truth is wiggly and the noise is low, so the more flexible fits do the best.

Nonlinear Model

```
set.seed(12345)
```

```
## Simulate x and y based on a known function
fun3 <- function(x) -(x-80)*(x-45)*(x-25)/15^3+10
x <- runif(50,0,100)
y <- fun3(x) + rnorm(50)
```

```
## Plot linear regression and splines
par(mfrow=c(1,2))
plot(x, y, xlab="X", ylab="Y")
```

```
plot(x, y, xlab="X", ylab="Y")
lines(sort(x), fun3(sort(x)), col=1, lwd=2)
abline(lm(y~x)$coef, col="orange", lwd=2)
lines(smooth.spline(x,y, df=5), col="blue", lwd=2)
lines(smooth.spline(x,y, df=23), col="green", lwd=2)
legend("topright", lty=1, col=c(1, "orange", "blue", "green"),
       legend=c("True", "df = 1", "df = 5", "df =23"),lwd=2)
```

Nonlinear Model

```
set.seed(45678)
```

```
## Simulate training and test data (x, y)
tran.x <- runif(50,0,100)
test.x <- runif(50,0,100)
tran.y <- fun3(tran.x) + rnorm(50)
test.y <- fun3(test.x) + rnorm(50)
```

```
## Compute MSE along with different df
df <- 2:40
MSE <- matrix(0, length(df), 2)
for (i in 1:length(df)) {
    tran.fit <- smooth.spline(tran.x, tran.y, df=df[i])
    MSE[i,1] <- mean((tran.y - predict(tran.fit, tran.x)$y)^2)
    MSE[i,2] <- mean((test.y - predict(tran.fit, test.x)$y)^2)
}
```

Nonlinear Model

```
## Plot both test and training errors
matplot(df, MSE, type="l", col=c("gray", "red"),
        xlab="Flexibility", ylab="Mean Squared Error",
        lwd=2, lty=1)
abline(h=1, lty=2)
legend("top", lty=1, col=c("red", "gray"),lwd=2,
       legend=c("Test MSE", "Training MSE"))
abline(v=df[which.min(MSE[,1])], lty=3, col="gray")
abline(v=df[which.min(MSE[,2])], lty=3, col="red")
```

```
matplot(df, MSE, type="l", col=c("gray", "red"),
        xlab="Flexibility", ylab="Mean Squared Error",
        lwd=2, lty=1, ylim=c(0,3), xlim=c(4,20))
abline(h=1, lty=2)
abline(v=df[which.min(MSE[,2])], lty=3, col="red")
```

Bias-Variance Trade-off

- Suppose that we fit a model $\hat{f}(X)$ to training data, and let (x_0, y_0) be a test observation drawn from the population.
- If the true model is

$$Y = f(X) + \epsilon$$

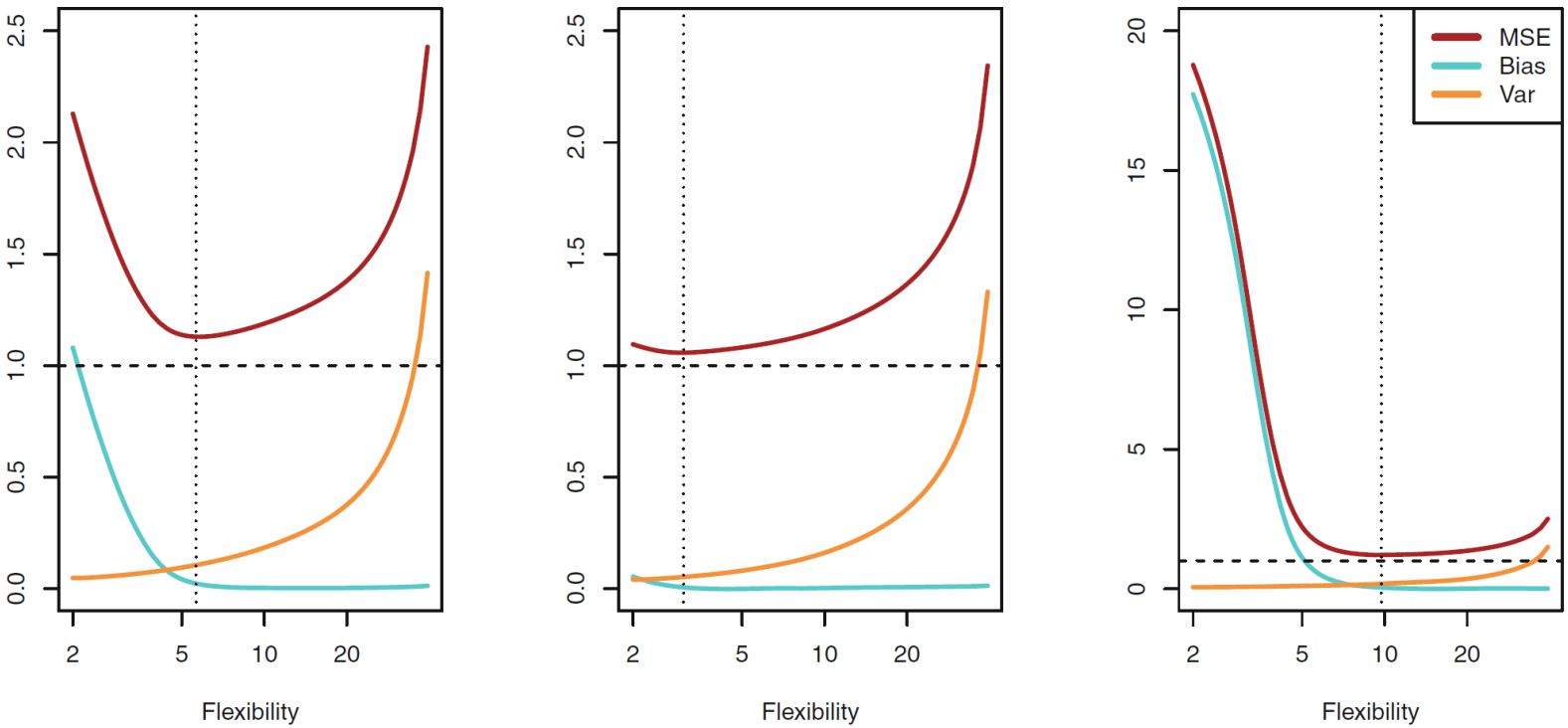
with $f(x) = E(Y|X = x)$, then

$$E\left(y_0 - \hat{f}(x_0)\right)^2 = \text{Var}\left(\hat{f}(x_0)\right) + \left[\text{Bias}(\hat{f}(x_0))\right]^2 + \text{Var}(\epsilon)$$

where $\text{Bias}(\hat{f}(x_0)) = E[\hat{f}(x_0)] - f(x_0)$.

- Typically as the flexibility of $\hat{f}$ increases, its variance increases, and its bias decreases. So choosing the flexibility based on average test error amounts to a bias-variance trade-off.

Bias-Variance Trade-off



- Squared bias (blue curve), variance (orange curve), $\mathrm{Var}(\epsilon)$ (dashed line), and test MSE (red curve).

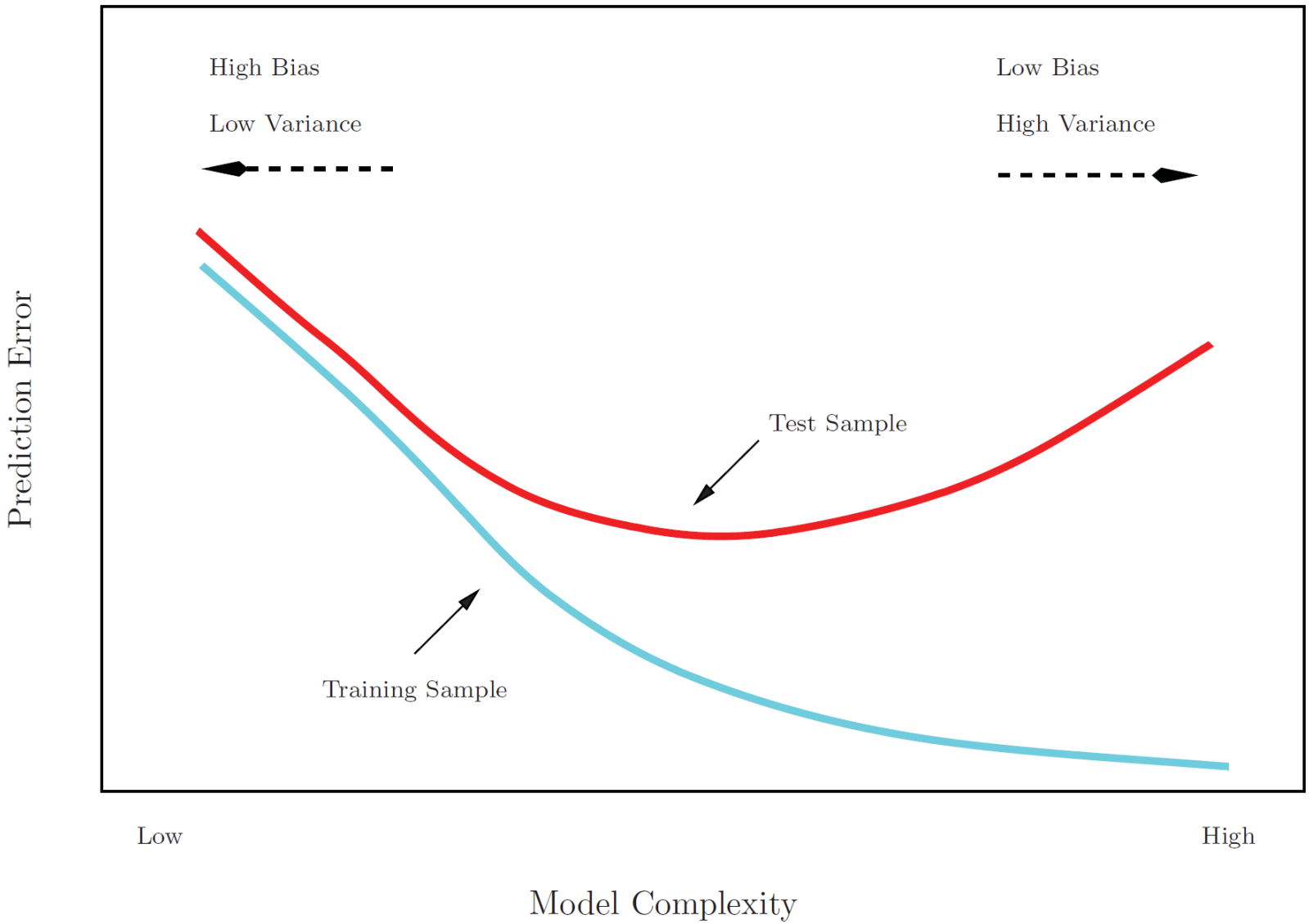
Bias-Variance Trade-off

- Good test set performance of a statistical learning method requires low variance as well as low squared bias.
- Trade-off: it is easy to obtain a method with extremely low bias but high variance or a method with very low variance but high bias.
- In a real-life situation in which f is unobserved, it is generally not possible to explicitly compute the test MSE, bias, or variance for a statistical learning method.
- We should always keep the bias-variance trade-off in mind to select the best statistical learning method.

Training Error versus Test error

- The test error is the average error that results from using a statistical learning method to predict the response on a new observation, one that was not used in training the method.
- In contrast, the training error can be easily calculated by applying the statistical learning method to the observations used in its training data.
- But the training error rate often is quite different from the test error rate, and in particular the former can dramatically underestimate the latter.
- In absence of a large designated test set to directly estimate the test error rate, a number of techniques can be used to estimate this quantity using available training data.

Training-set versus Test-set Performance



More on Prediction-error Estimates

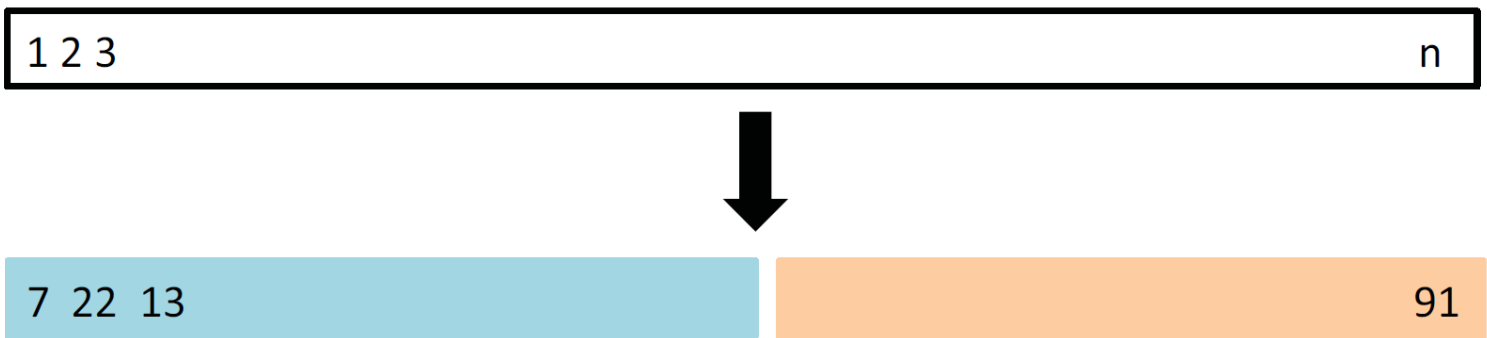
- Best solution: a large designated test set. Often not available.
- Some methods make a mathematical adjustment to the training error rate in order to estimate the test error rate. These include the C_p statistic, AIC and BIC.
- Here we instead consider a class of methods that estimate the test error by holding out a subset of the training observations from the fitting process, and then applying the statistical learning method to those held out observations.
  - Validation set approach
  - K-fold cross-validation
  - Leave-one-out cross-validation (LOOCV)

Validation Set Approach

- Here we randomly divide the available set of samples into two parts: a training set and a validation or hold-out set.
- The model is fit on the training set, and the fitted model is used to predict the responses for the observations in the validation set.
- The resulting validation set error provides an estimate of the test error. This is typically assessed using Mean Squared Error (MSE) in the case of a quantitative response and misclassification rate in the case of a qualitative (or binary) response.

Validation Set Approach

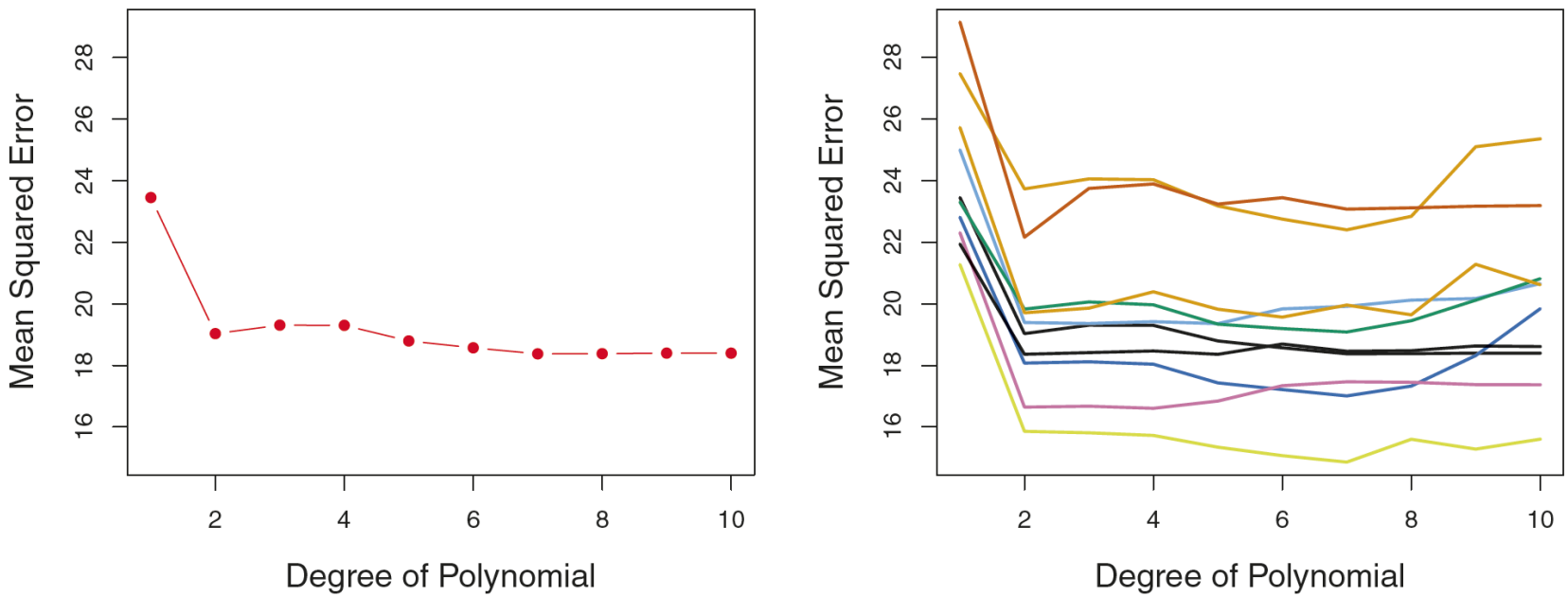
- A random splitting into two halves: left part is training set, right part is validation set.



- In next example, we want to compare linear vs. higher-order polynomial terms in a linear regression, using the validation set approach.

Example: Auto Data

- We randomly split the 392 observations into two sets, a training set containing 196 of the data points, and a validation set containing the remaining 196 observations.



Left panel shows single split and right panel shows multiple splits

Auto Data

```
library(ISLR)
data(Auto)
str(Auto)
summary(Auto)
```

```
mpg <- Auto$mpg
horsepower <- Auto$horsepower
```

```
dg <- 1:9
u <- order(horsepower)
```

```
par(mfrow=c(3,3))
for (k in 1:length(dg)) {
    g <- lm(mpg ~ poly(horsepower, dg[k]))
    plot(mpg~horsepower, col=2, pch=20, xlab="Horsepower",
        ylab="mpg", main=paste("dg =", dg[k]))
    lines(horsepower[u], g$fit[u], col="darkblue", lwd=3)
}
```

Auto Data: Single Split

```
set.seed(1)
n <- nrow(Auto)
```

```
## training set
tran <- sample(n, n/2)
```

```
MSE <- NULL
for (k in 1:length(dg)) {
    g <- lm(mpg ~ poly(horsepower, dg[k]), subset=tran)
    MSE[k] <- mean((mpg - predict(g, Auto))[-tran]^2)
}
```

```
par(mfrow=c(1,3))
plot(dg, MSE, type="b", col=2, xlab="Degree of Polynomial",
     ylab="Mean Squared Error", ylim=c(15,30), lwd=2, pch=19)
abline(v=which.min(MSE), lty=2)
```

Auto Data: Multiple Splits

```
K <- 10
MSE <- matrix(0, length(dg), K)
```

```
for (i in 1:K) {
    tran <- sample(392, 196)
    for (k in 1:length(dg)) {
        g <- lm(mpg ~ poly(horsepower, dg[k]), subset=tran)
        MSE[k, i] <- mean((mpg - predict(g, Auto))[-tran]^2)
    }
}
matplot(dg, MSE, type="l", xlab="Degree of Polynomial", lty=1,
        ylab="Mean Squared Error", col=1:10, ylim=c(15,30))
```

```
avg <- apply(MSE, 1, mean)
plot(dg, avg, type="b", col=2, xlab="Degree of Polynomial",
     ylab="Mean Squared Error", ylim=c(15,30), lwd=2, pch=19)
abline(v=which.min(avg), lty=2)
```

Drawbacks of Validation Set Approach

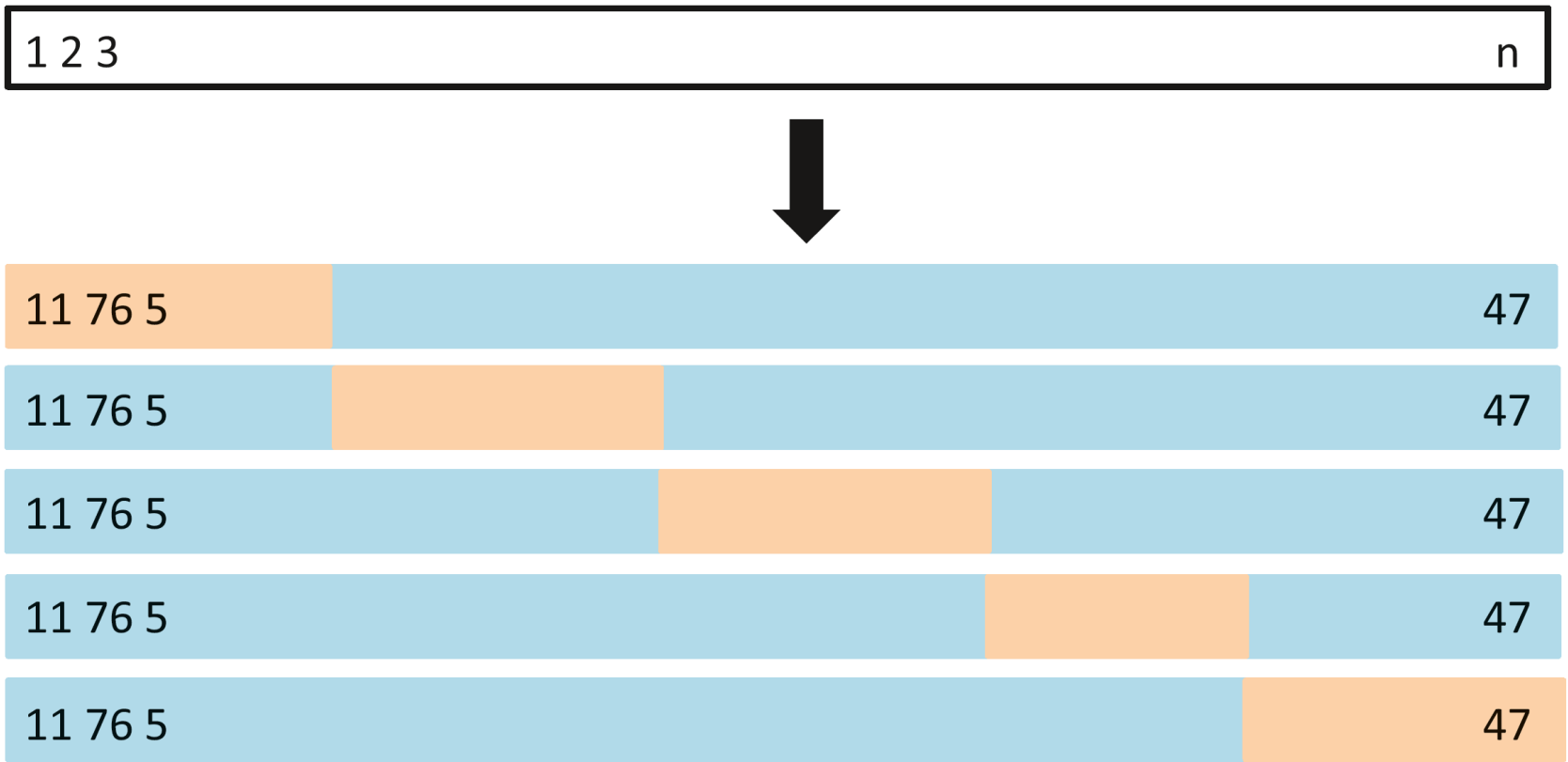
- The validation estimate of the test error can be highly variable, depending on precisely which observations are included in the training set and which observations are included in the validation set.
- In the validation approach, only a subset of the observations – those that are included in the training set rather than in the validation set are used to fit the model.
- This suggests that the validation set error may tend to incorrectly estimate the test error for the model fit on the entire data set.

K-fold Cross-validation

- K-fold Cross-validation is widely used approach for estimating test error.
- Estimates can be used to select the best model, and to give an idea of the test error of the final chosen model.
- Idea is to randomly divide the data into K equal-sized parts. We leave out part k, fit the model to the other $K-1$ parts (combined training set), and then obtain predictions for the left-out kth part (test set).
- This is done in turn for each part $k = 1, 2, \cdots, K$, and then the results are combined.

The Validation Process

- Divide data into K roughly equal-sized parts ($K = 5$ here)



Cross-validation Error for Quantitative Outcomes

- Suppose that y_i is a quantitative value.
- Let the K parts be C_1, C_2, ..., C_K, where C_k denotes the indices of the observations in part k. There are n_k observations in part k.
- Compute Cross-validation Error (CVE)

$$\text{CVE} = \frac{1}{n} \sum_{k=1}^{K} n_k MSE_k$$

where

$$MSE_k = \frac{1}{n_k} \sum_{i \in C_k} (y_i - \hat{y}_i^{[-k]})^2$$

and $\hat{y}_i^{[-k]}$ is the fit for the observation i, obtained from the data with part k removed.

Cross-validation Error for Binary Outcomes

- Suppose that $y_i = 1$ for cases and $y_i = 0$ for controls.
- Cross-validation Error (CVE) can be computed from
  - Deviance

$$\text{CVE} = \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in C_k} -2 \left(y_i \log \hat{p}_i^{[-k]} + (1 - y_i) \log(1 - \hat{p}_i^{[-k]}) \right),$$

    where $\hat{p}_i^{[-k]}$ is the probability of $y_i = 1$ for the observation i, obtained from the data with part k removed.
  - Classification error

$$\text{CVE} = \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in C_k} I \left(y_i - \hat{y}_i^{[-k]} \right),$$

    where $\hat{y}_i^{[-k]}$ is the fit for the observation i, obtained from the data with part k removed.

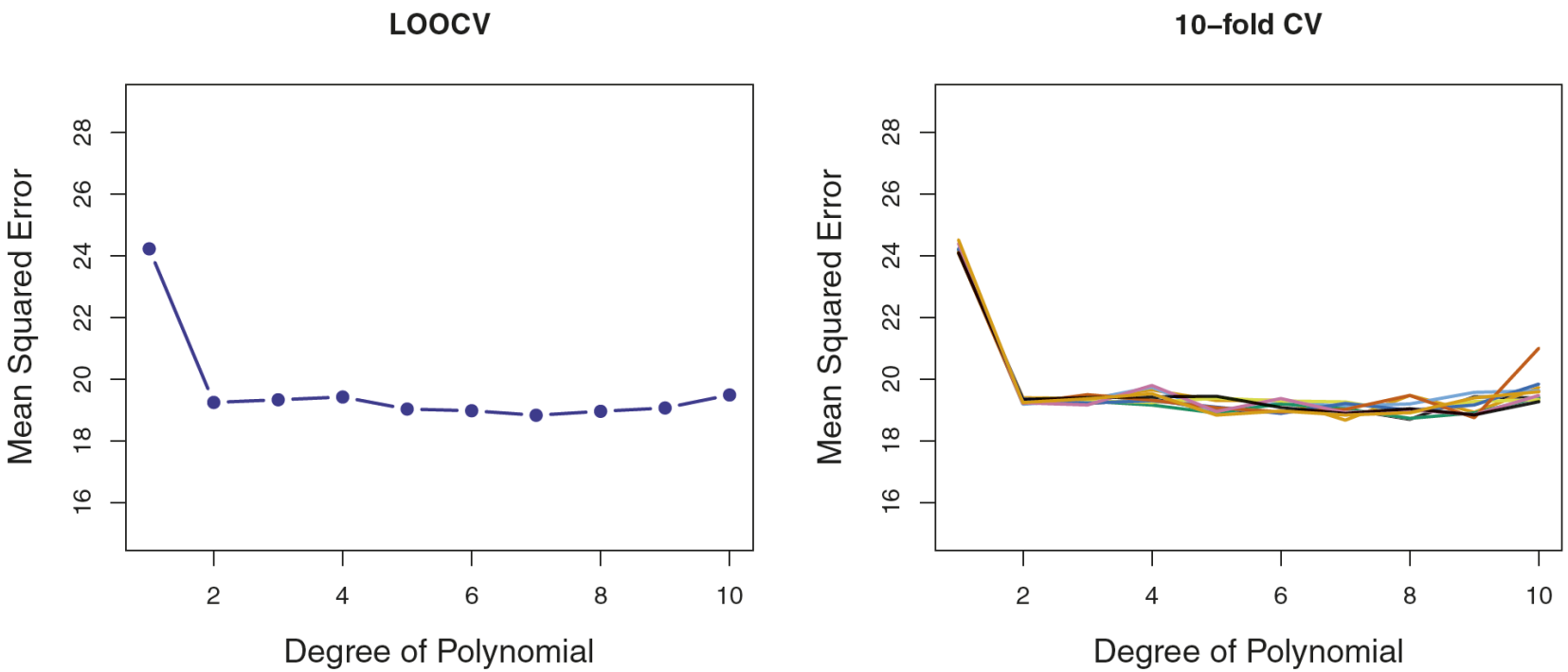
Special Case of LOOCV

- Setting $K = n$ yields leave-one out cross-validation (LOOCV).
- With least-squares of linear or polynomial regression, an amazing shortcut makes the cost of LOOCV the same as that of a single model fit. The following formula holds:

$$\text{CV error} = \frac{1}{n}\sum_{i=1}^{n}\left(\frac{y_i - \hat{y}_i}{1 - h_i}\right)^2$$

  where $\hat{y}_i$ is the ith fitted value from the original least squares fit, and h_i is the leverage. This is like the ordinary MSE, except the ith residual is divided by $1 - h_i$.
- LOOCV sometimes useful, but typically doesn't shake up the data enough. The estimates from each fold are highly correlated and hence their average can have high variance. A better choice is $K = 5$ or 10.

Example: Auto Data



Left panel shows LOOCV and right panel shows 10-fold CV

Auto Data : LOOCV

```
n <- nrow(Auto)
dg <- 1:9
MSE <- matrix(0, n, length(dg))
```

```
for (i in 1:n) {
    for (k in 1:length(dg)) {
        g <- lm(mpg ~ poly(horsepower, k), subset=(1:n)[-i])
        MSE[i, k] <- mean((mpg - predict(g, Auto))[i]^2)
    }
}
aMSE <- apply(MSE, 2, mean)
```

```
par(mfrow=c(1, 2))
plot(dg, aMSE, type="b", col="darkblue",
     xlab="Degree of Polynomial", ylab="Mean Squared Error",
     ylim=c(18,25), lwd=2, pch=19)
abline(v=which.min(aMSE), lty=2)
```

Auto Data : LOOCV

```
ncv <- NULL
for (k in 1:length(dg)) {
    g <- lm(mpg ~ poly(horsepower, k))
    ncv[k] <- mean((g$res/(1-influence(g)$hat))^2)
}
lines(dg, ncv, col=2, lty=2, lwd=2)
```

```
K <- 10     ## 10-fold cross validation
MSE <- matrix(0, n, length(dg))
```

```
set.seed(54321)
u <- sample(rep(seq(K), length=n))
table(u)
```

Auto Data: K-fold CV

```
for (k in 1:K) {
    tran <- which(u!=k)
    test <- which(u==k)
    for (i in 1:length(dg)) {
        g <- lm(mpg ~ poly(horsepower, i), subset=tran)
        MSE[test, i] <- (mpg - predict(g, Auto))[test]^2
    }
}
CVE <- apply(MSE, 2, mean)
```

```
plot(dg, CVE, type="b", col="darkblue",
     xlab="Degree of Polynomial", ylab="Mean Squared Error",
     ylim=c(18,25), lwd=2, pch=19)
abline(v=which.min(CVE), lty=2)
```

```
N <- 9      ## Number of K-fold CV replications
KCV <- matrix(0, length(dg), N)
```

Auto Data: K-fold CV

```
set.seed(1234)
for (j in 1:N) {
    MSE <- matrix(0, n, length(dg))
    u <- sample(rep(seq(K), length=n))
    for (k in 1:K) {
        tran <- which(u!=k)
        test <- which(u==k)
        for (i in 1:length(dg)) {
            g <- lm(mpg ~ poly(horsepower, i), subset=tran)
            MSE[test, i] <- (mpg - predict(g, Auto))[test]^2
        }
    }
    KCV[,j] <- apply(MSE, 2, mean)
}
```

```
dev.off()
matplot(dg, KCV, type="l", xlab="Degree of Polynomial", lty=1,
        ylab="MSE", ylim=c(18,25), main="10-fold CV")
apply(KCV, 2, which.min)
```

R Package 'boot': Cross Validation

```
library(boot)
set.seed(101010)
```

```
## Leave-one-out CV
MSE <- NULL
for (i in 1:length(dg)) {
    glm.fit <- glm(mpg ~ poly(horsepower ,i))
    MSE[i] <- cv.glm(Auto, glm.fit)$delta[1]
}
plot(dg, MSE, type="b", col="darkblue", ylim=c(15,29),
     xlab="Degree of Polynomial", ylab="MSE", lwd=2, pch=19)
```

```
## K-fold cross validation
K <- 10
KCV <- NULL
for (i in 1:length(dg)) {
    glm.fit <- glm(mpg ~ poly(horsepower ,i))
    KCV[i] <- cv.glm(Auto, glm.fit, K=K)$delta[1]
}
lines(dg, KCV, col=2, lwd=2, type="b", pch=19, lty=2)
```