Lecture 2: Prediction

Part I: Splines, Additive Models
Part II: Model Selection and Validation

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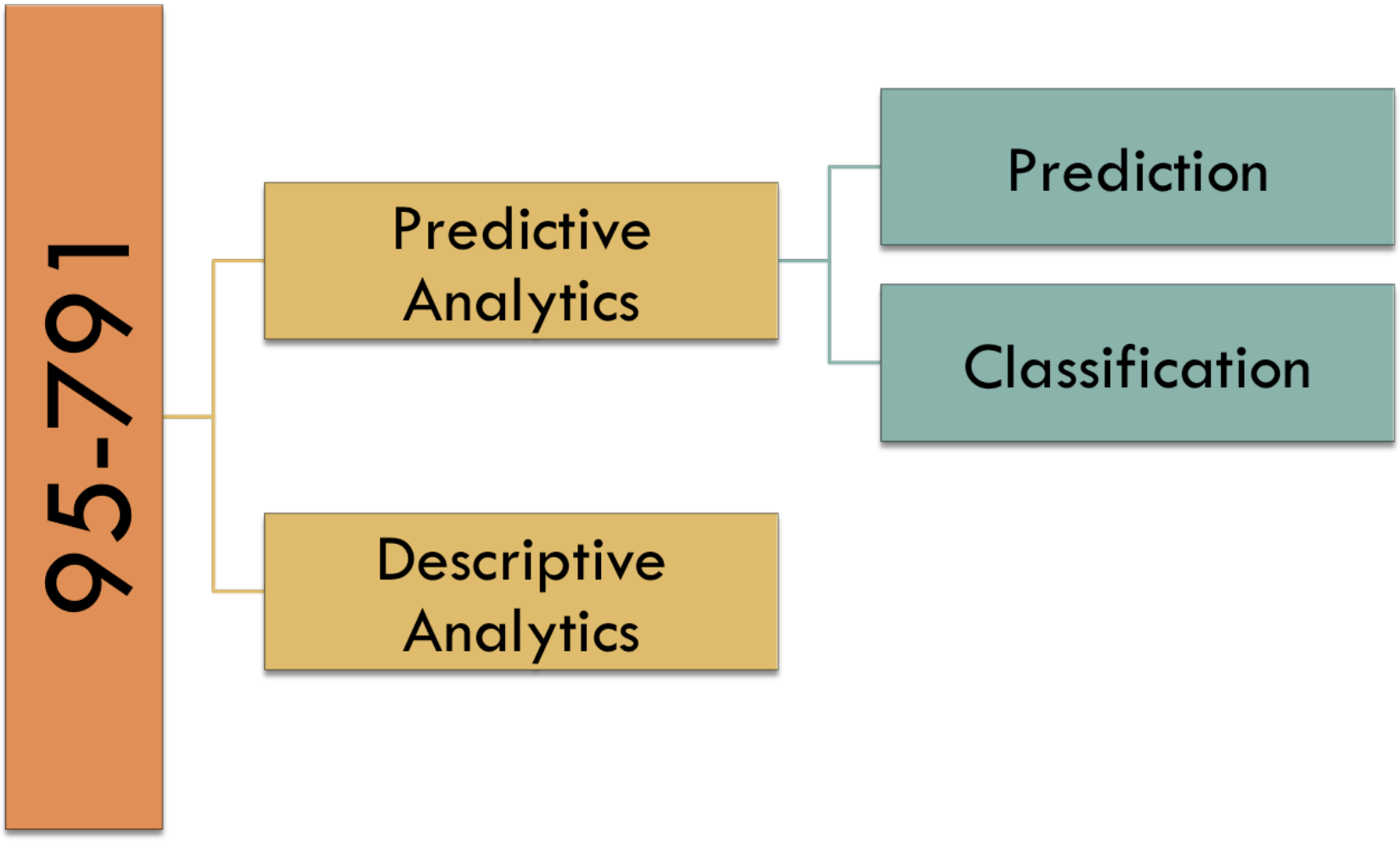
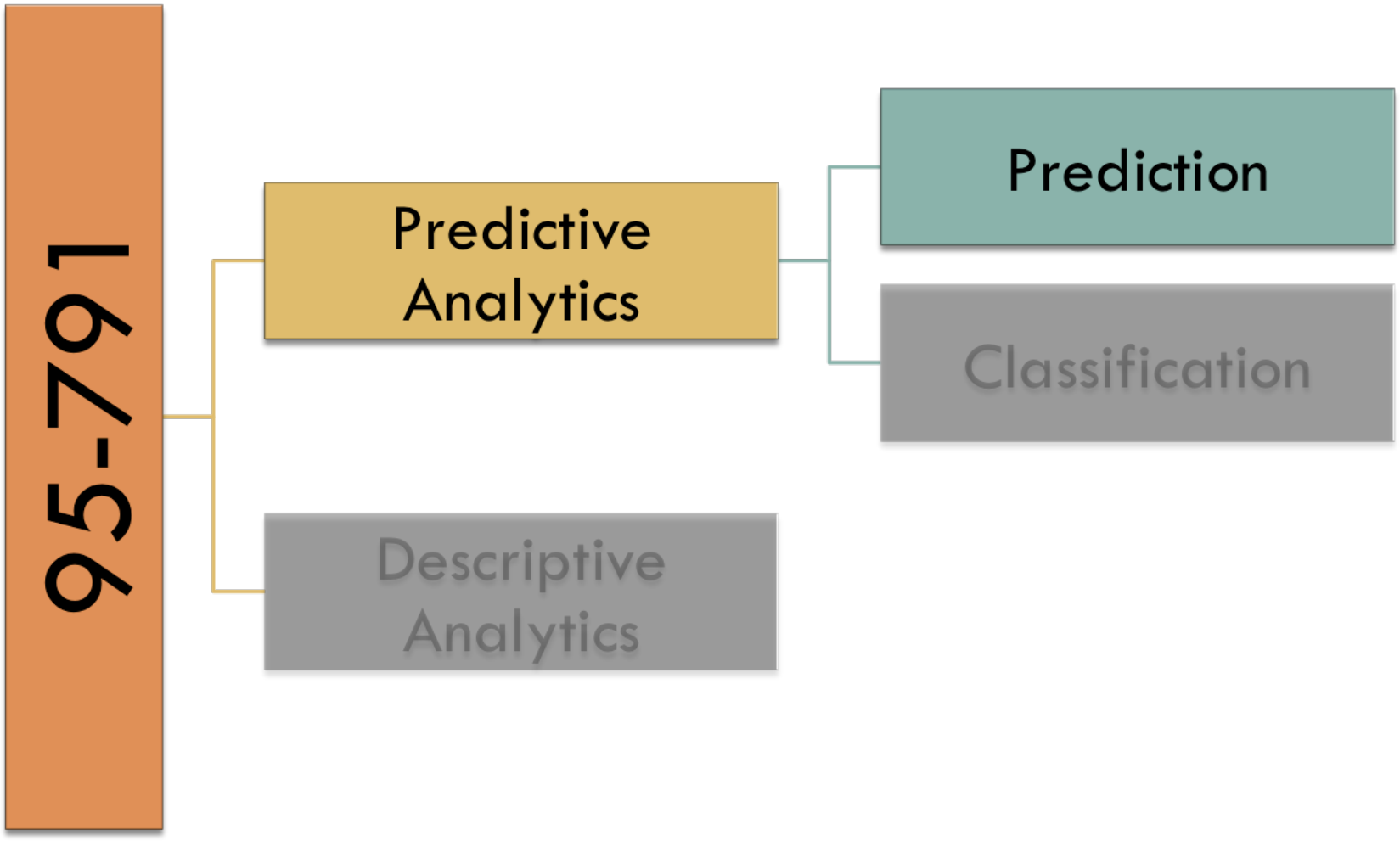
95-791: Data Mining

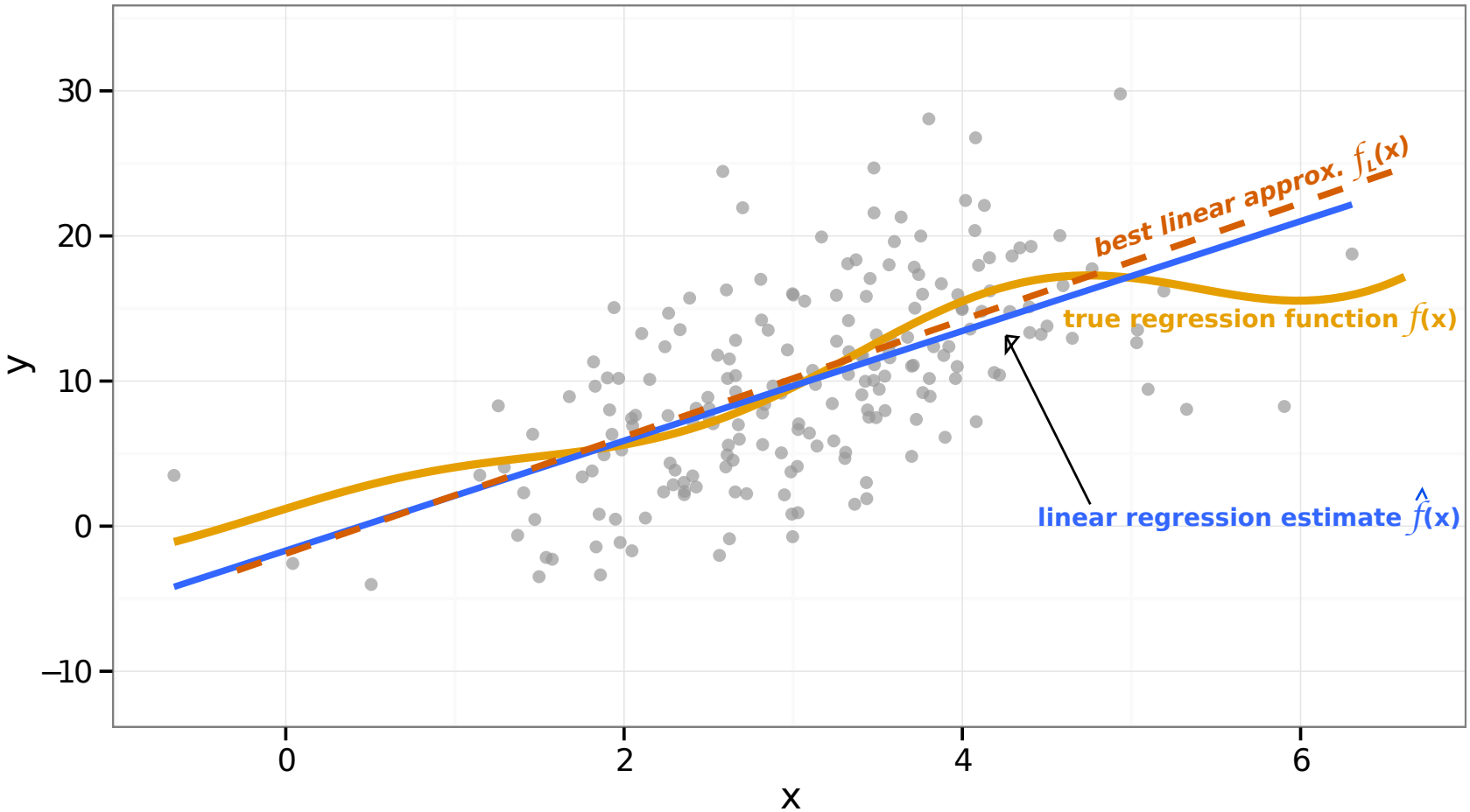
Course Roadmap



Course Roadmap



Recap of last class



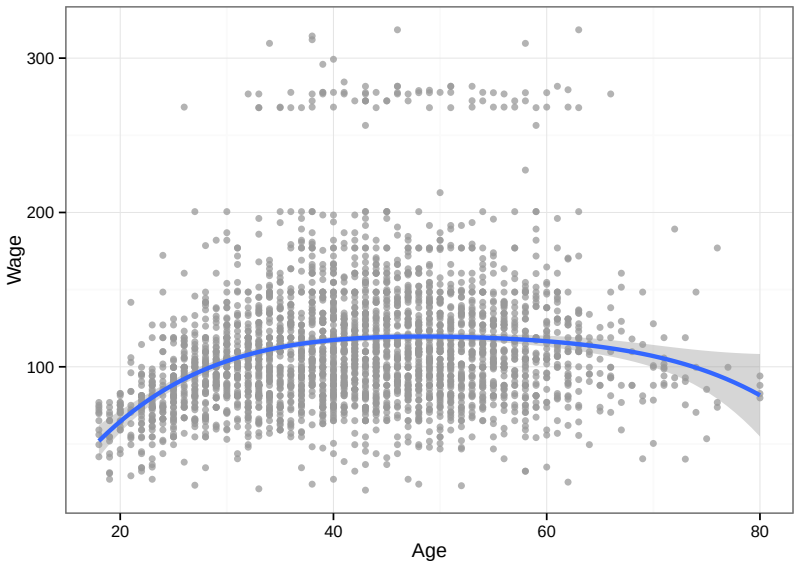
- The goal of prediction is to estimate the true, unknown regression function, f

Recap of last class

- Linear regression imposes two key restrictions on the model: We assume the relationship between the response Y and the predictors $X_1, \ldots, X_p$ is:
  1. Linear
  2. Additive
- The truth is almost never linear; but often the linearity and additivity assumptions are *good enough*
- When we think linearity might not hold, we can try…
  - Polynomials
  - Step functions
  - Splines
  - Local regression
  - Generalized additive models
- When we think the additivity assumption doesn't hold, we can incorporate interaction terms
- These variants offer increased flexibility, while retaining much of the ease and interpretability of ordinary linear regression

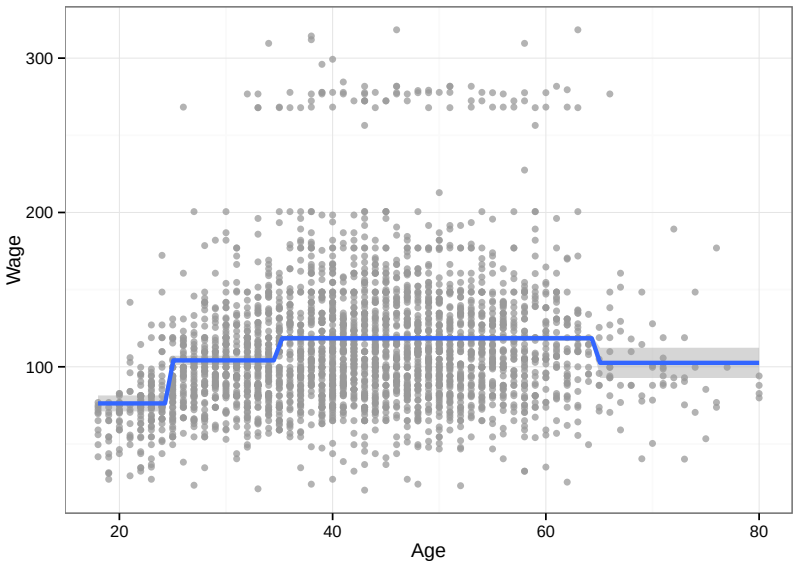
Recap of last class

Polynomials




```
lm(wage ~ poly(age, 4), data = Wage)
```

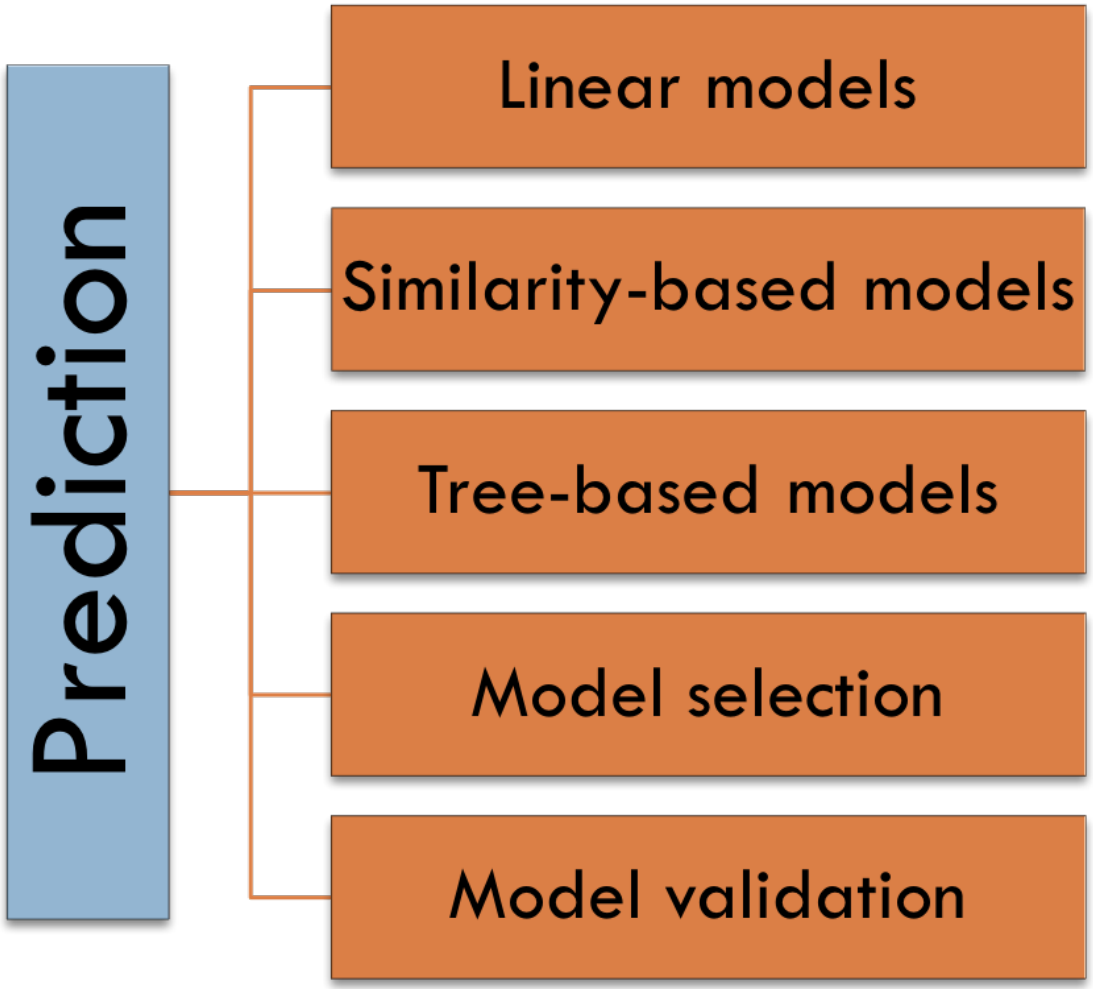
Step Functions



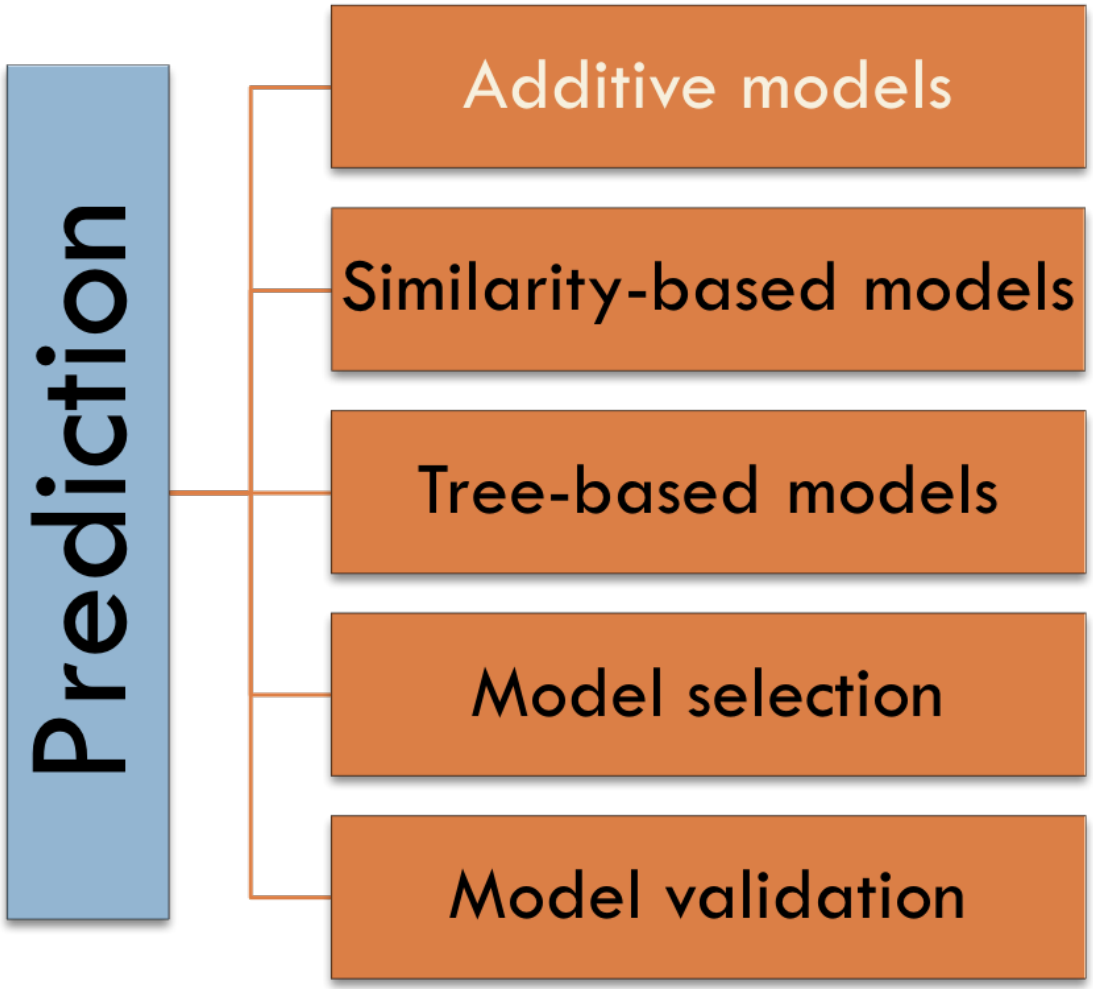

```
lm(wage ~ cut(age,
    breaks = c(-Inf, 25, 35, 65, Inf)),
    data = Wage)
```

- We can think of polynomials and step functions as simple forms of feature engineering
- These extensions of linear regression enable us to fit much more flexible models

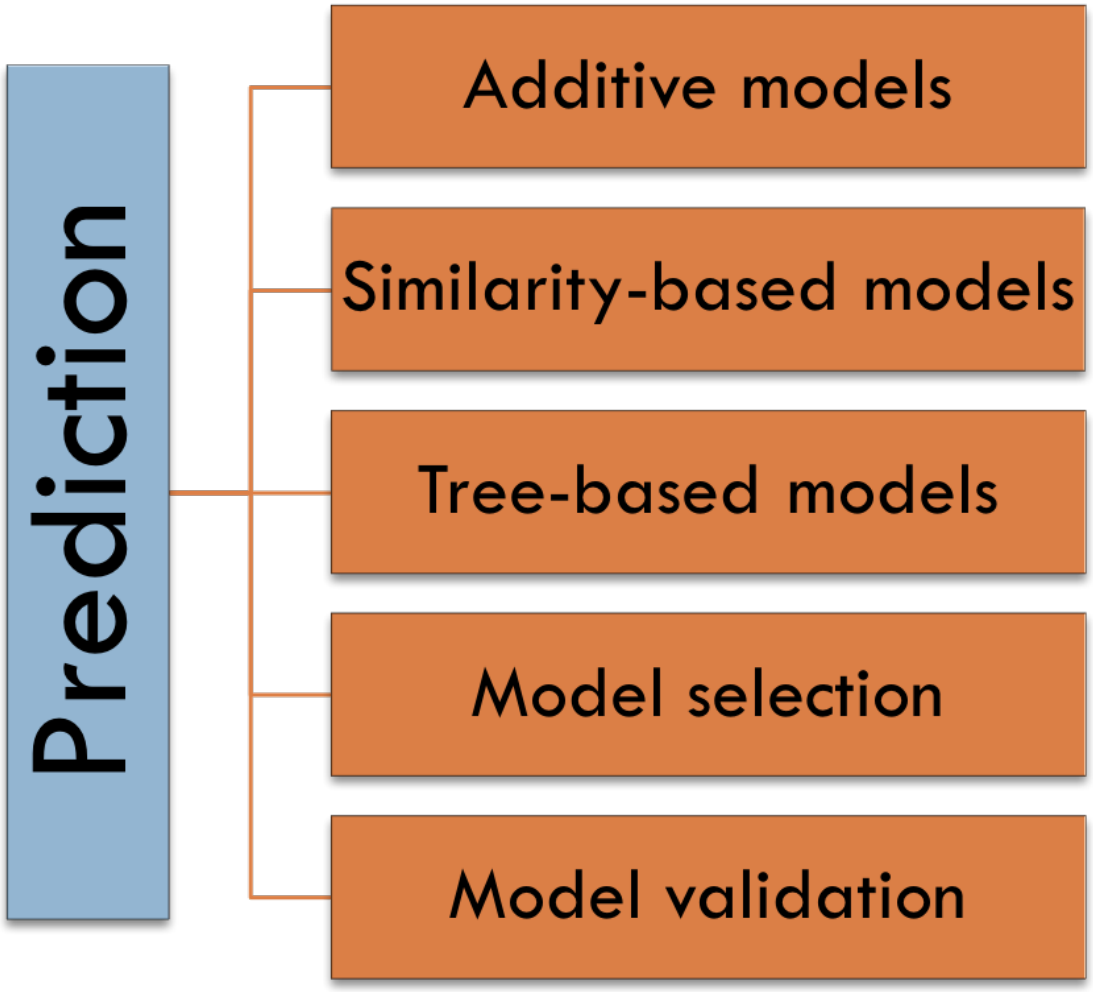
Prediction topics: Part I



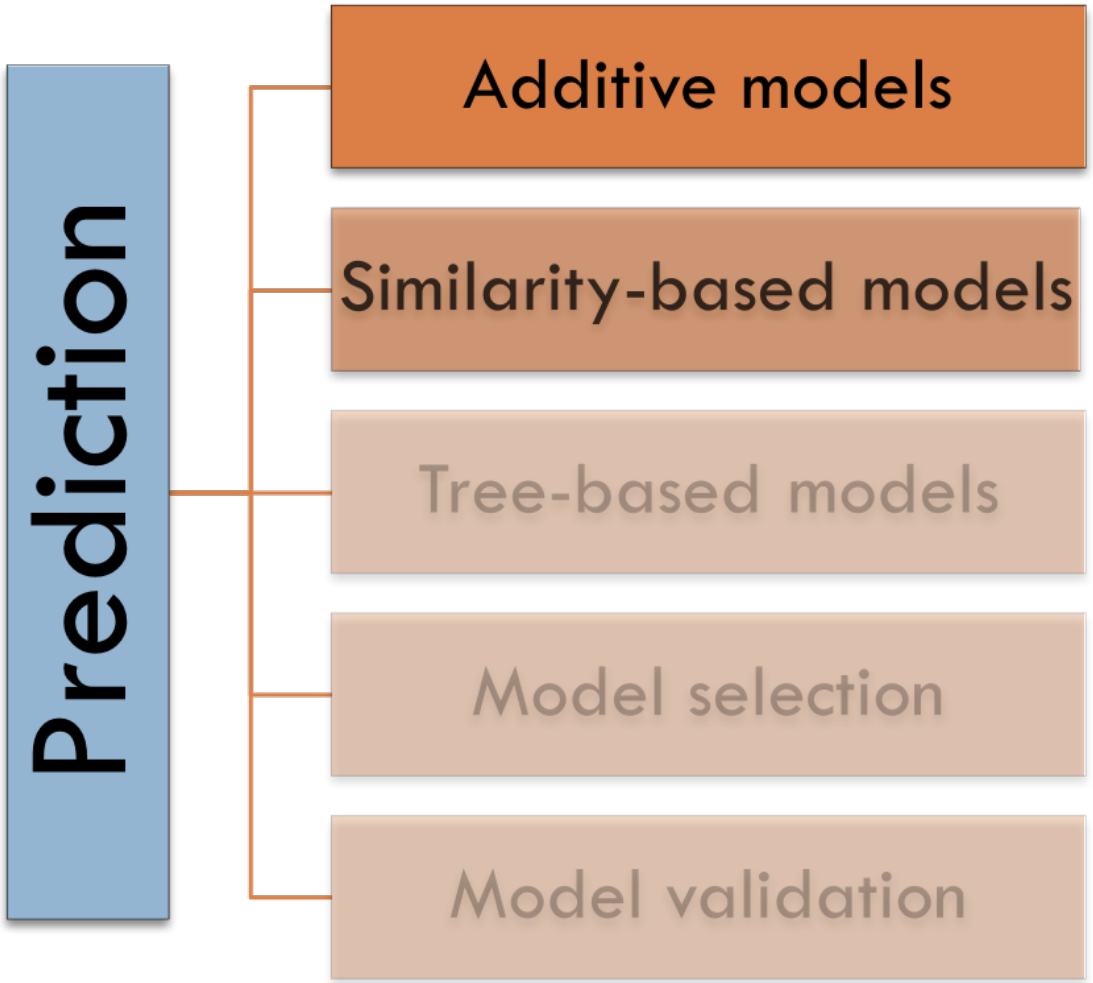
Prediction topics: Part I



Prediction topics: Part I



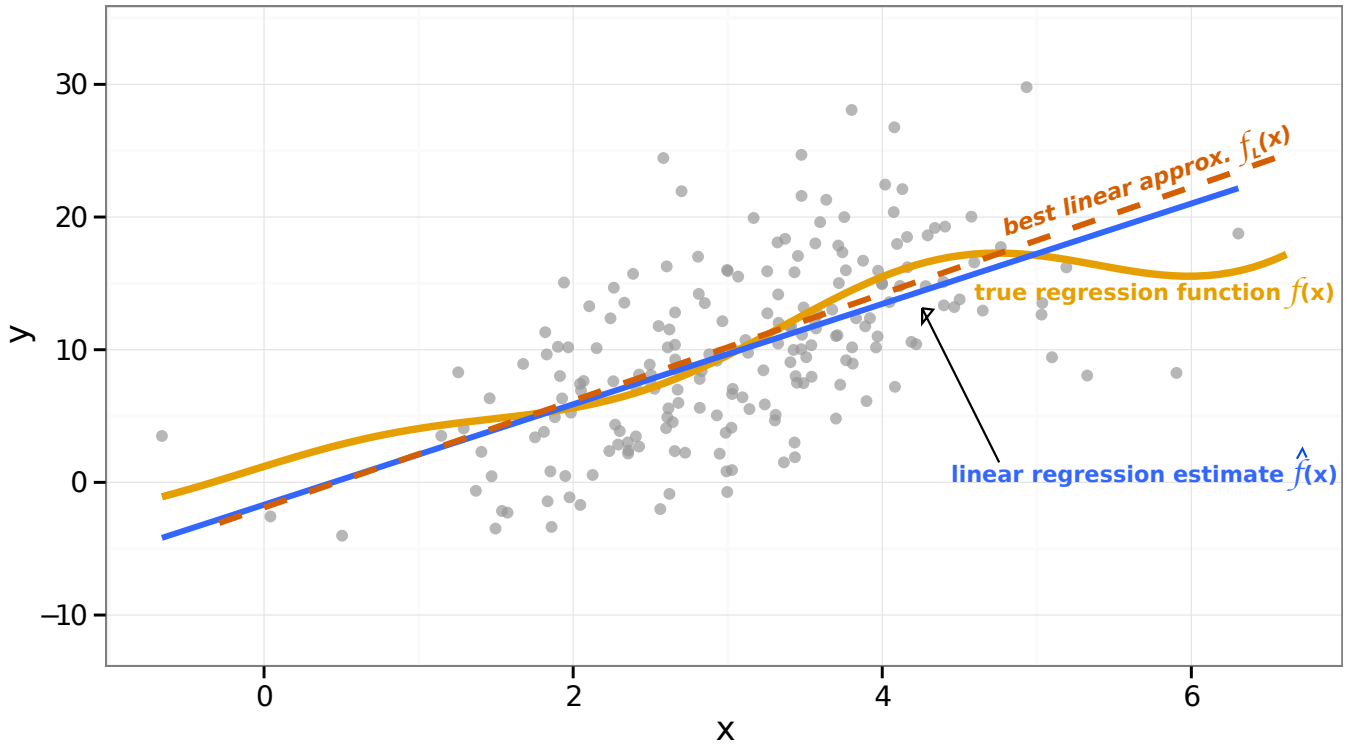
Prediction topics: Part I



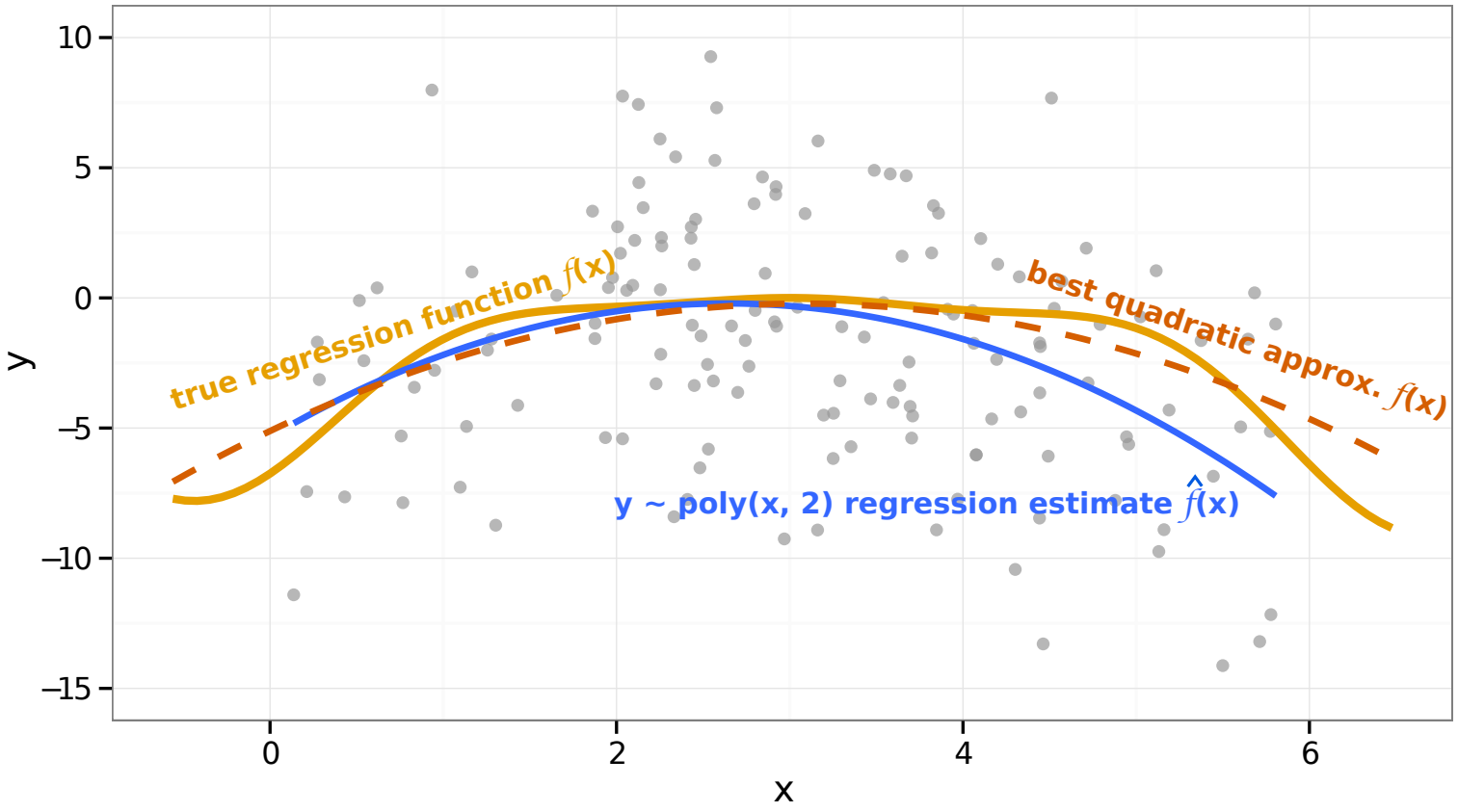
Agenda for Part I

- Piecewise polynomial fits
- Splines
- Additive models

Some motivation



- If the true regression function f is non-linear, ordinary linear regression cannot estimate it consistently
- No matter how much data you get, the best ordinary linear regression can do is converge to the best linear approximation to f



- The same problem persists with polynomial regression
- No matter how much data you get, the best degree-k polynomial regression can do is converge to the best degree-k approximation to f

Consistency

Consistent estimator

An estimator $\hat{f}(x)$ is consistent if, as our sample size grows, $\hat{f}(x)$ *converges* to the true regression function $f(x) = \mathbb{E}(Y \mid X = x)$

- Unless $f(x)$ is a polynomial of degree $\leq k$, degree-k polynomial regression is not consistent

Q: Can we get a consistent estimator of a generic regression function f?

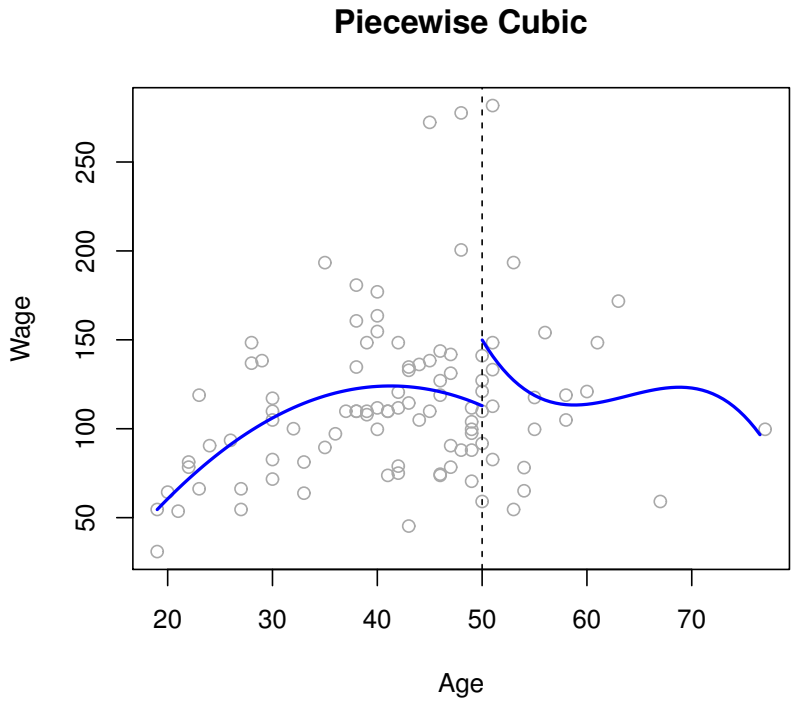
A: If we're willing to assume f is *smooth*, then **YES**

Use **splines**!

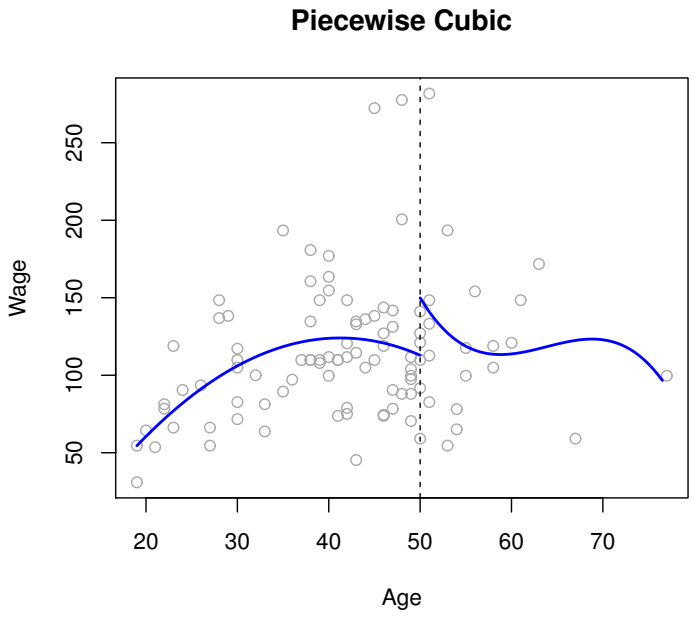
Piecewise polynomials

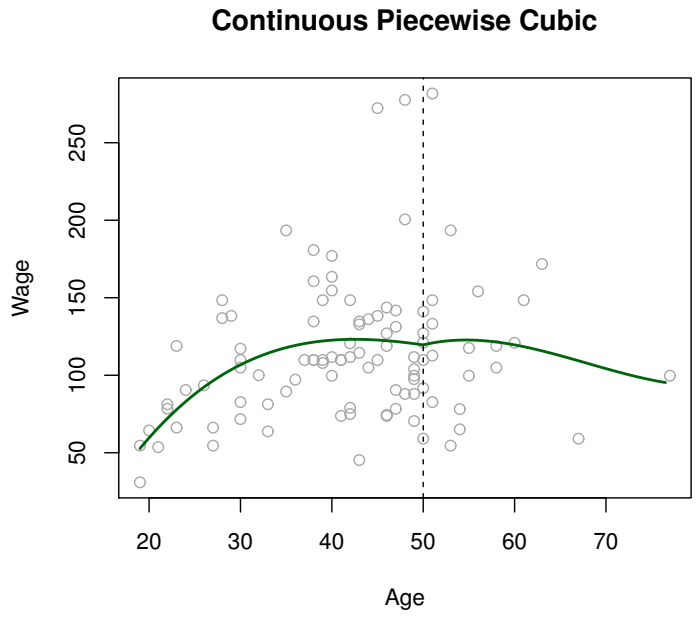
To understand splines, we first need to understand piecewise polynomials

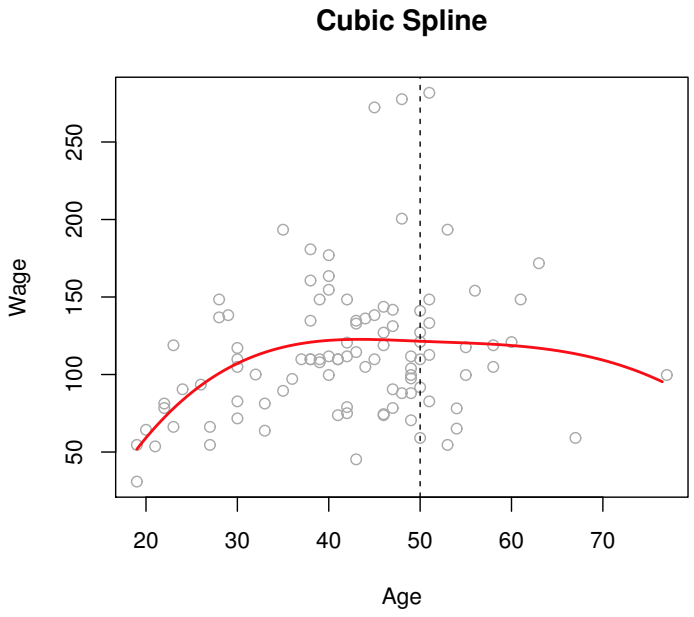
- We can think of step functions as piecewise constant models
- It's easy to generalize this idea to:
  - Piecewise linear
  - Piecewise quadratic …
  - Piecewise polynomial

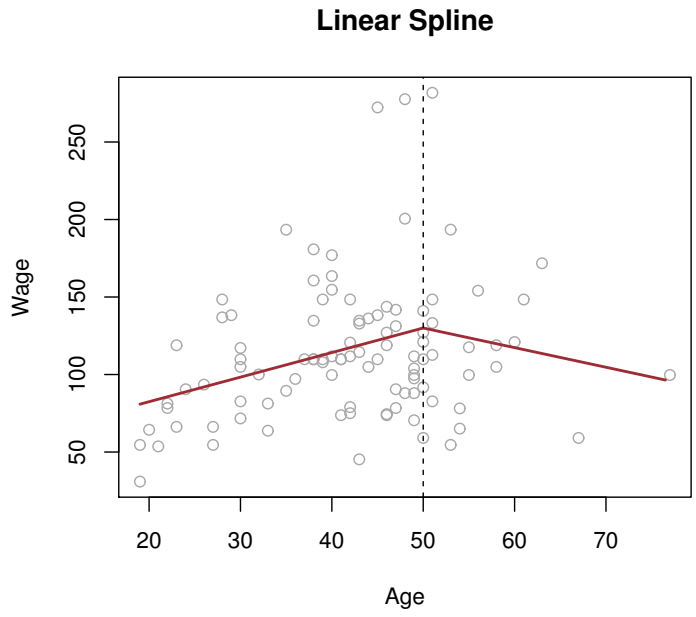


Piecewise Polynomial vs. Regression Splines

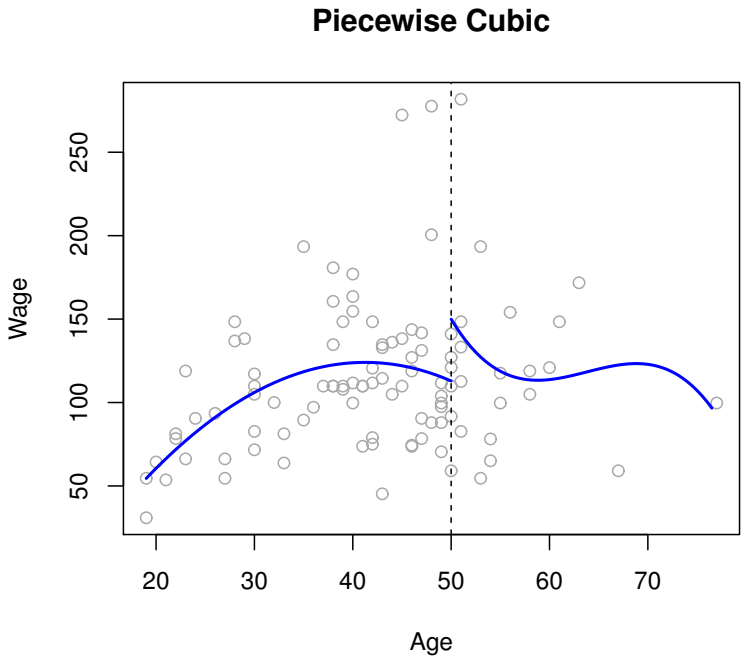


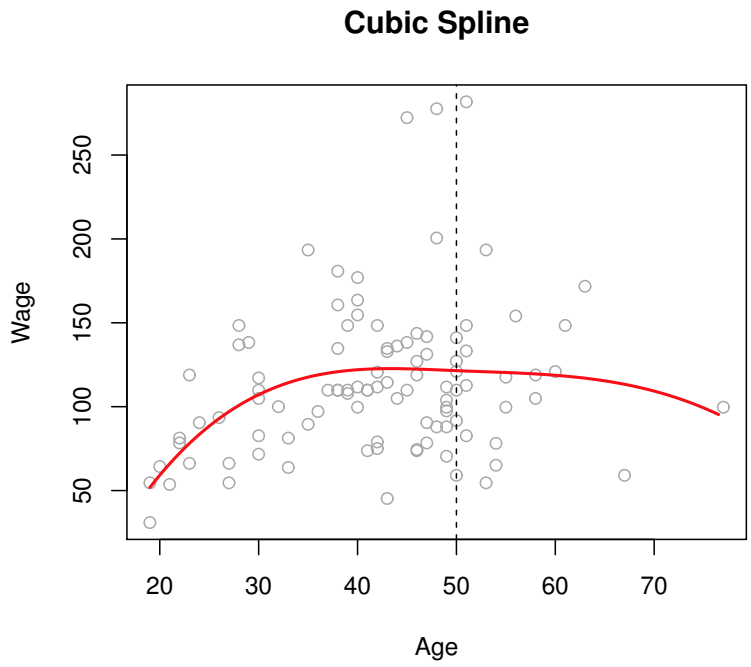






Piecewise polynomial vs. Regression splines





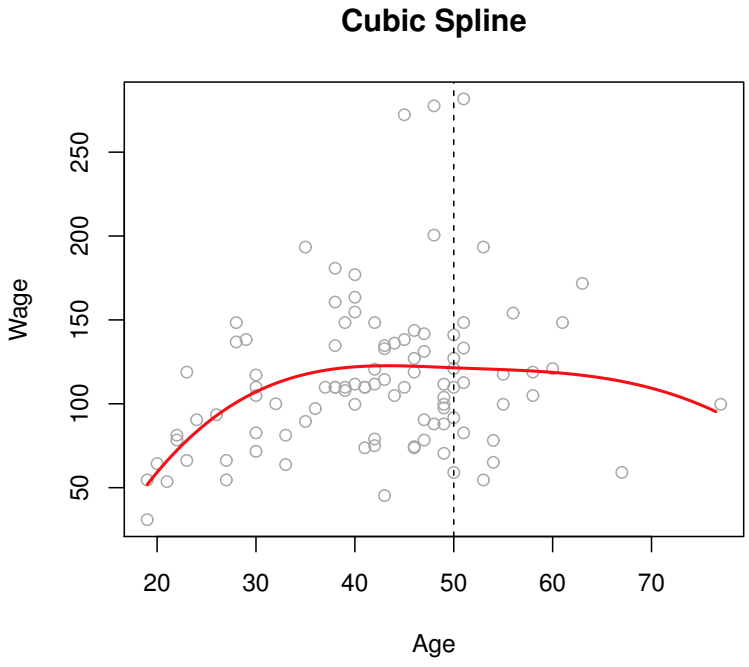
1 break at Age $= 50$

1 knot at Age $= 50$

Definition: Cubic spline

A cubic spline with knots at x-values $\xi_1, \ldots, \xi_K$ is a continuous piecewise cubic polynomial with *continuous derivates* and *continuous second derivatives* at each knot.

Cubic Splines



- Turns out, cubic splines are sufficiently flexible to *consistently* estimate smooth regression functions f
- You can use higher-degree splines, but *there's no need to*
- To fit a cubic spline, we just need to pick the knots

Polynomial regression vs. Cubic splines

- In polynomial regression, we had to choose the degree
- For cubic splines, we need to choose the knots
- **Q:** How *complex* is a cubic spline with K knots?
- *Paraphrasing*…A cubic spline with K knots is as complex as a polynomial of degree ____?
  - Turns out, there exist functions $b_k(x)$[1] such that a cubic spline with K knots can be modeled as

$$y = \beta_0 + \beta_1 b_1(x) + \beta_2 b_2(x) + \cdots \beta_{K+3} b_{K+3}(x) + \epsilon$$

- So…**A:** A *cubic spline* with K knots is as complex as a polynomial of degree $K + 3$.

[1] See ISLR pg. 273 for details

Degrees of freedom

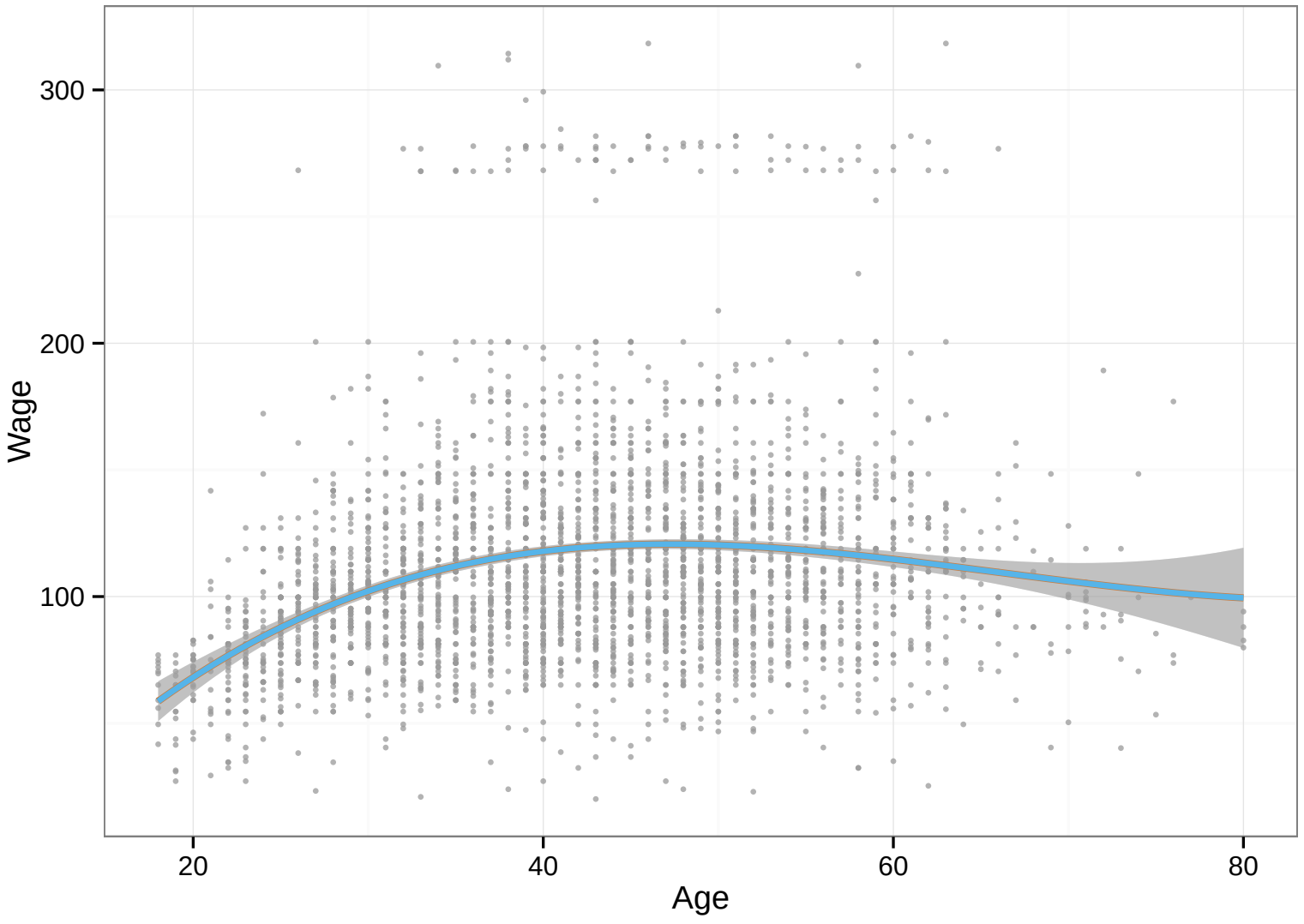
- Degrees of freedom capture the *complexity* of a regression model
- A linear regression model with p independent predictors is said to have p *degrees of freedom*[2]
- Take-away from the previous slide:

Model	# knots	Degrees of freedom
Regression, p predictors		p
Degree-k polynomial regression		k
Cubic spline	k	$k+3$
Degree-d Spline	k	$k+d$

- In the following slides, we compare *cubic splines* to *polynomial regression*, allowing each method the same degrees of freedom

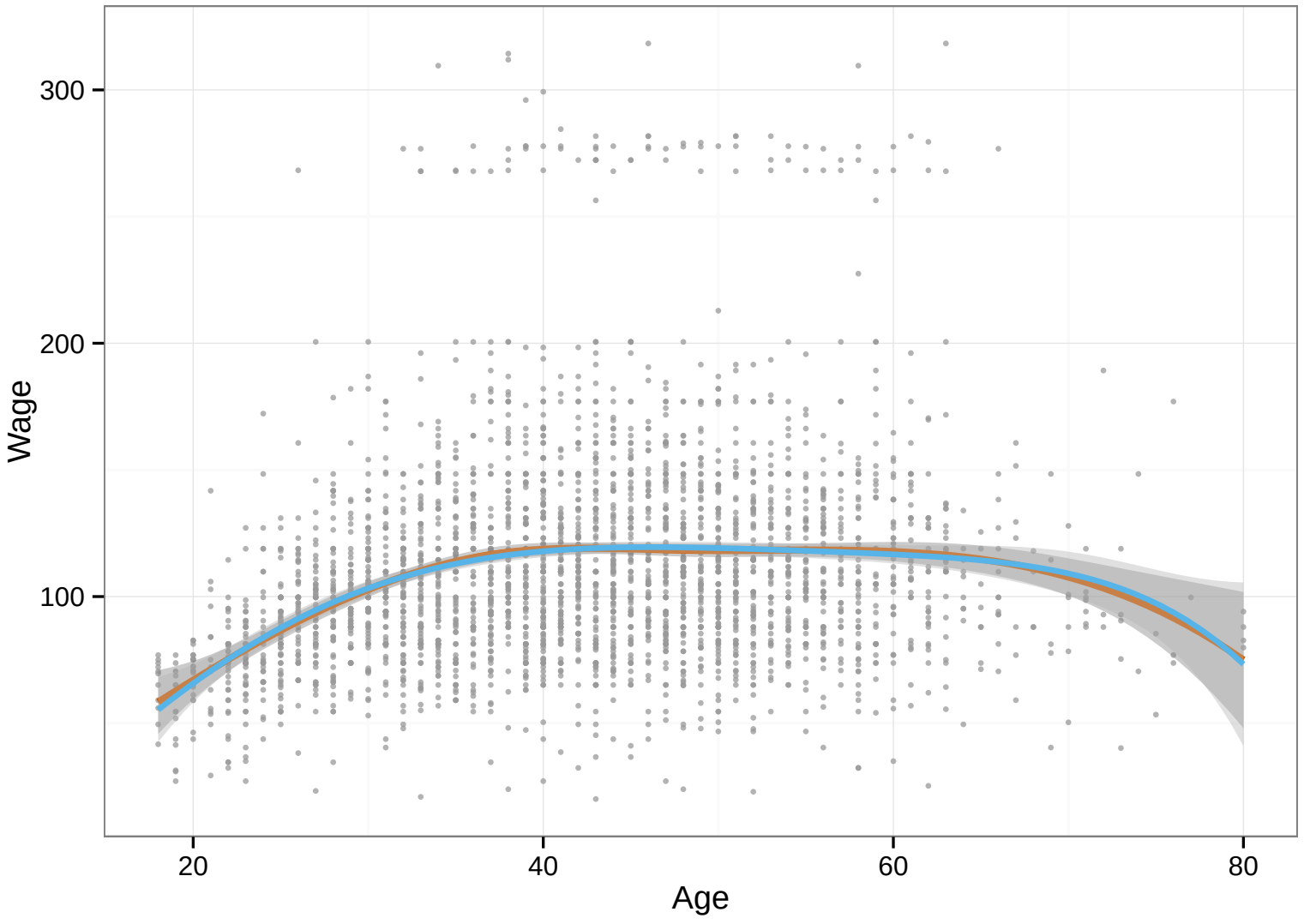
[2] Technically, $p+1$ if you count the intercept. To be consistent with R's `df` arguments, here we *do not* count the intercept.

Polynomial regression vs. Cubic splines




```
lm(wage ~ bs(age, df = 3))
lm(wage ~ poly(age, degree = 3))
```

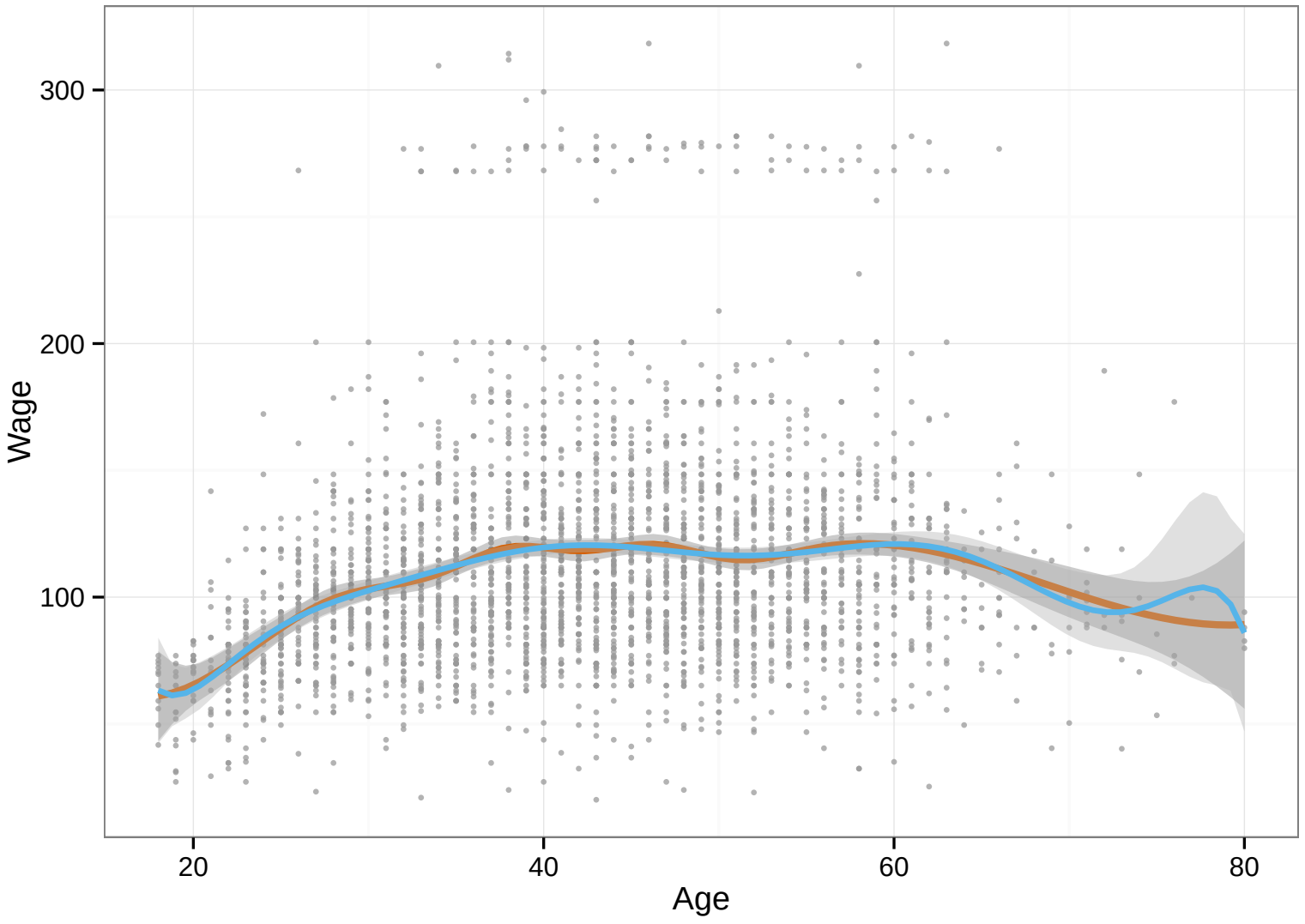
Polynomial regression vs. Cubic splines



`lm(wage ~ bs(age, df = 5))`

`lm(wage ~ poly(age, degree = 5))`

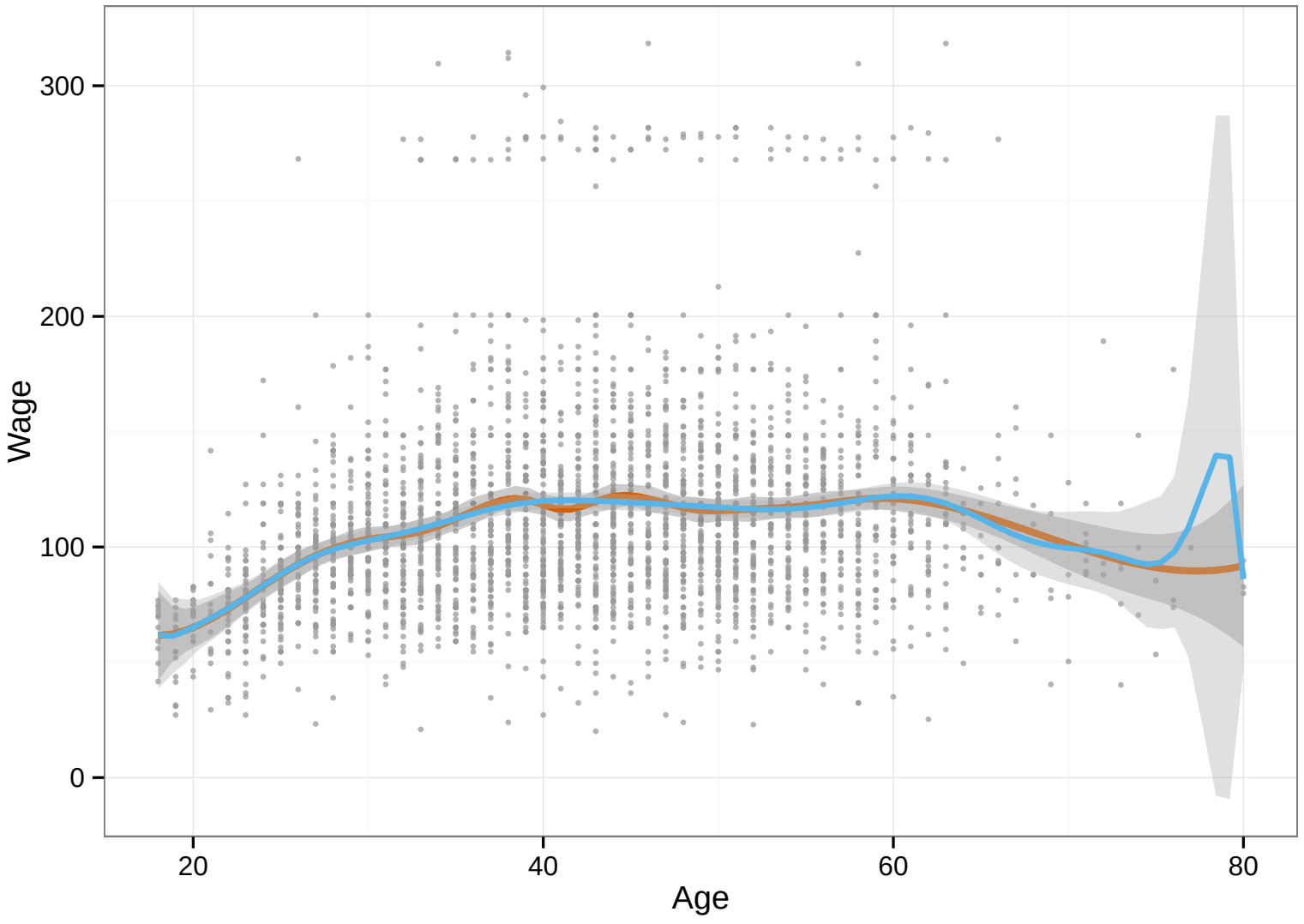
Polynomial regression vs. Cubic splines



`lm(wage ~ bs(age, df = 10))`

`lm(wage ~ poly(age, degree = 10))`

Polynomial regression vs. Cubic splines



`lm(wage ~ bs(age, df = 15))`

`lm(wage ~ poly(age, degree = 15))`

Natural Cubic Splines

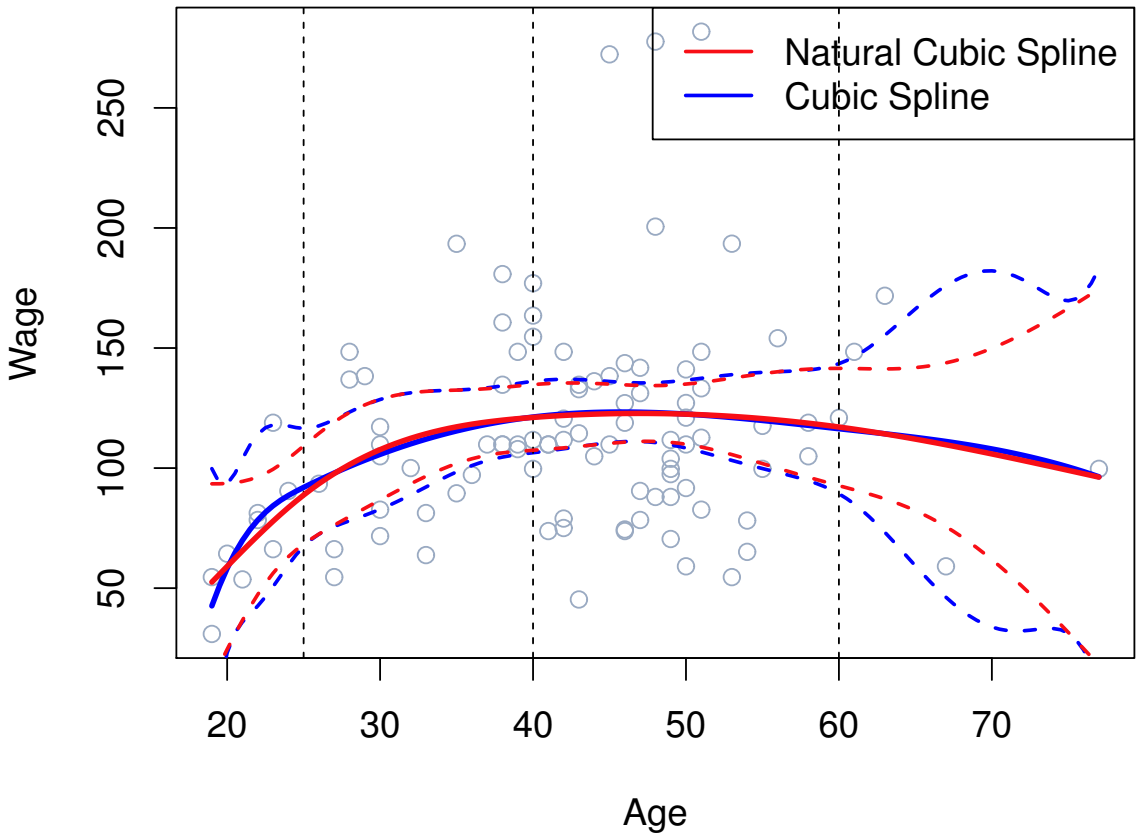


Figure: 7.4 from ISLR. Natural cubic splines are *cubic splines* that extrapolate linearly beyond the boundary knots. A NCS with K knots uses just $K + 1$ degrees of freedom — the same as a cubic spline with 2 *fewer knots*

Natural Cubic Splines vs Polynomial regression

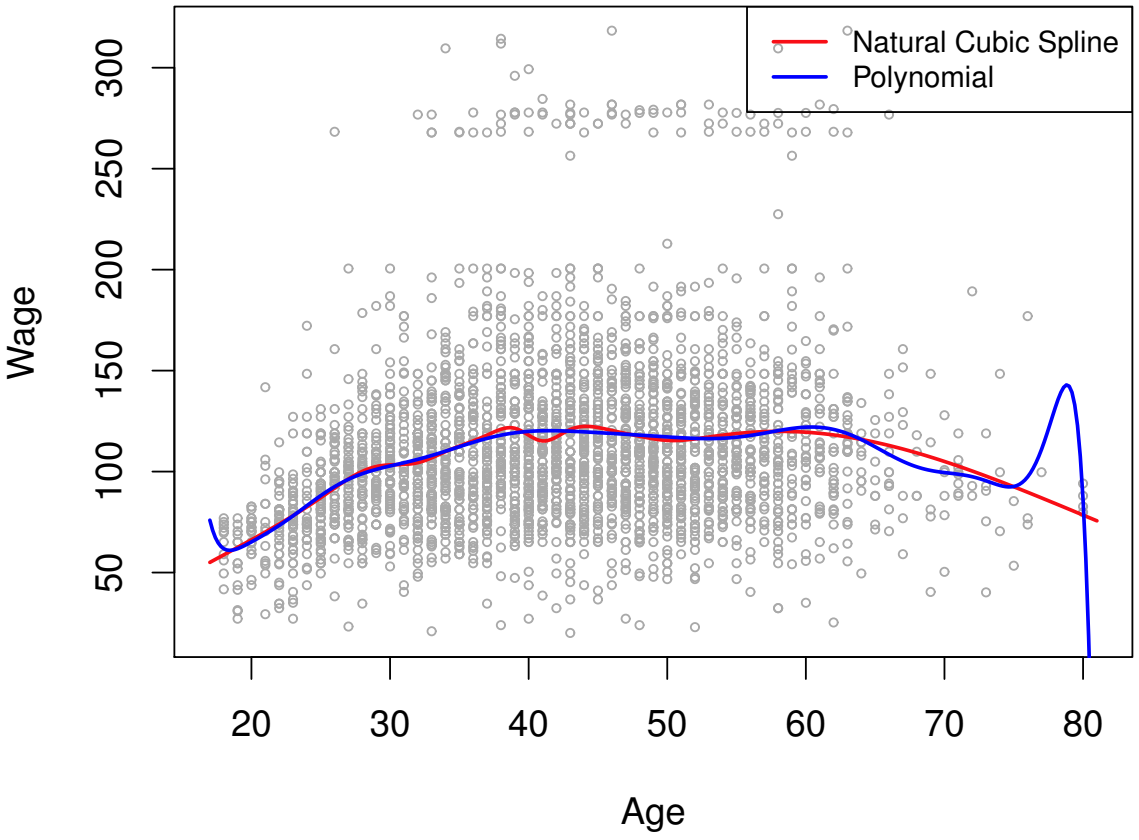
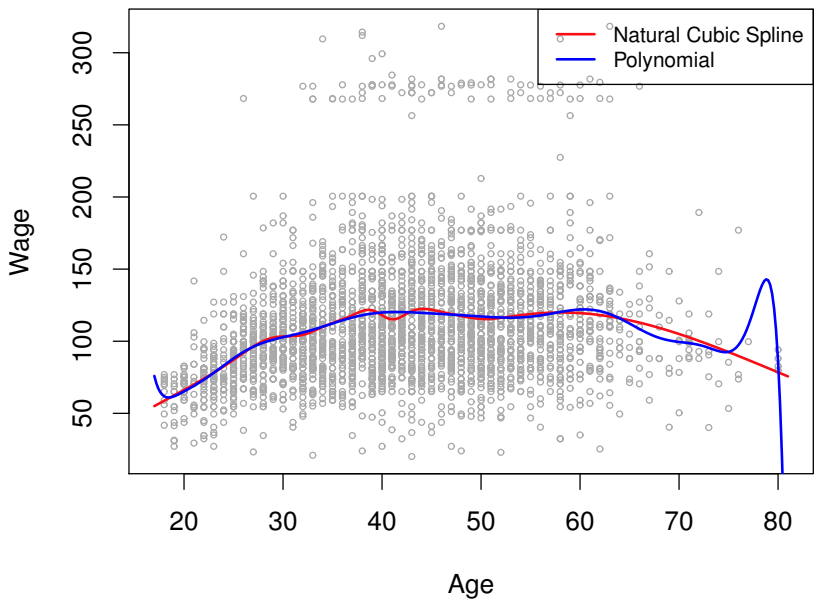


Figure: 7.7 from ISLR. Natural cubic splines are very nicely behaved at the tails of the data. Polynomial regression shows erratic behaviour. (14 degrees of freedom used for both)

Summary: Cubic Splines vs Polynomial regression



- Polynomial regression must use a high degree in order to produce flexible fits
- With splines, we can keep the degree fixed, an increase flexibility by adding knots
- Splines generally tend to be better behaved at the same level of *model complexity*

Knot placement: Rules of thumb

- Place more knots where f appears to be changing rapidly
- Place fewer knots where f appears to be slowly varying

R's defaults:

The most common way of specifying splines in **R** is in terms of the spline's degrees of freedom (df). **R** then places knots at suitably chosen *quantiles* of the x variable.

Model	**R** command	# internal knots
Cubic Spline	`~ bs(x, df)`	$\texttt{df} - 3$
Natural Cubic Spline	`~ ns(x, df)`	$\texttt{df} - 1$
Degree-d Spline	`~ bs(x, df, degree = d)`	$\texttt{df} - d$

- You may also specify the internal knots *manually* for `ns` and `bs` by specifying the `knots =` argument directly. E.g.,

```
lm(wage ~ bs(age, knots = c(25, 40, 60)), data = Wage)
```

Smoothing splines

- **Q:** What is the best way to *automatically* place knots?
- *Paraphrasing*…If I know how many degrees of freedom I want my spline to have, is there a method for automatically choosing the best locations for the knots?
- **A:** Smoothing splines

Smoothing splines

- The smoothing spline estimator is the solution $\hat{g}$ to the problem

$$\text{minimize} \underbrace{\sum_{i=1}^{n}(y_i - g(x_i))^2}_{\text{RSS}} + \underbrace{\lambda \int g''(t)^2 dt}_{\text{Roughness penalty}}$$

- This is a penalized regression problem[3]
- We're saying we want a function that:
  1. Fits the data well; and
  2. isn't too *wiggly*
- Large $\lambda \implies \hat{g}$ will have low variability (& higher bias)
- Small $\lambda \implies \hat{g}$ will have high variability (& lower bias)

How is this *at all* related to splines?

[3] We'll see more examples of penalized regression next class.

Smoothing splines

$$\text{minimize} \underbrace{\sum_{i=1}^{n}(y_i - g(x_i))^2}_{\text{RSS}} + \underbrace{\lambda \int g''(t)^2 dt}_{\text{Roughness penalty}} \qquad (*)$$

It turns out…

- The solution to $(*)$ is a natural cubic spline
- The solution has knots at every unique value of x
- The effective degrees of freedom of the solution is calculable
- $\lambda \longleftrightarrow df$

Coding tip: In **R** with the `gam` library you can use the syntax `s(x, df)` in your regression formula to fit a smoothing spline with `df` effective degrees of freedom.

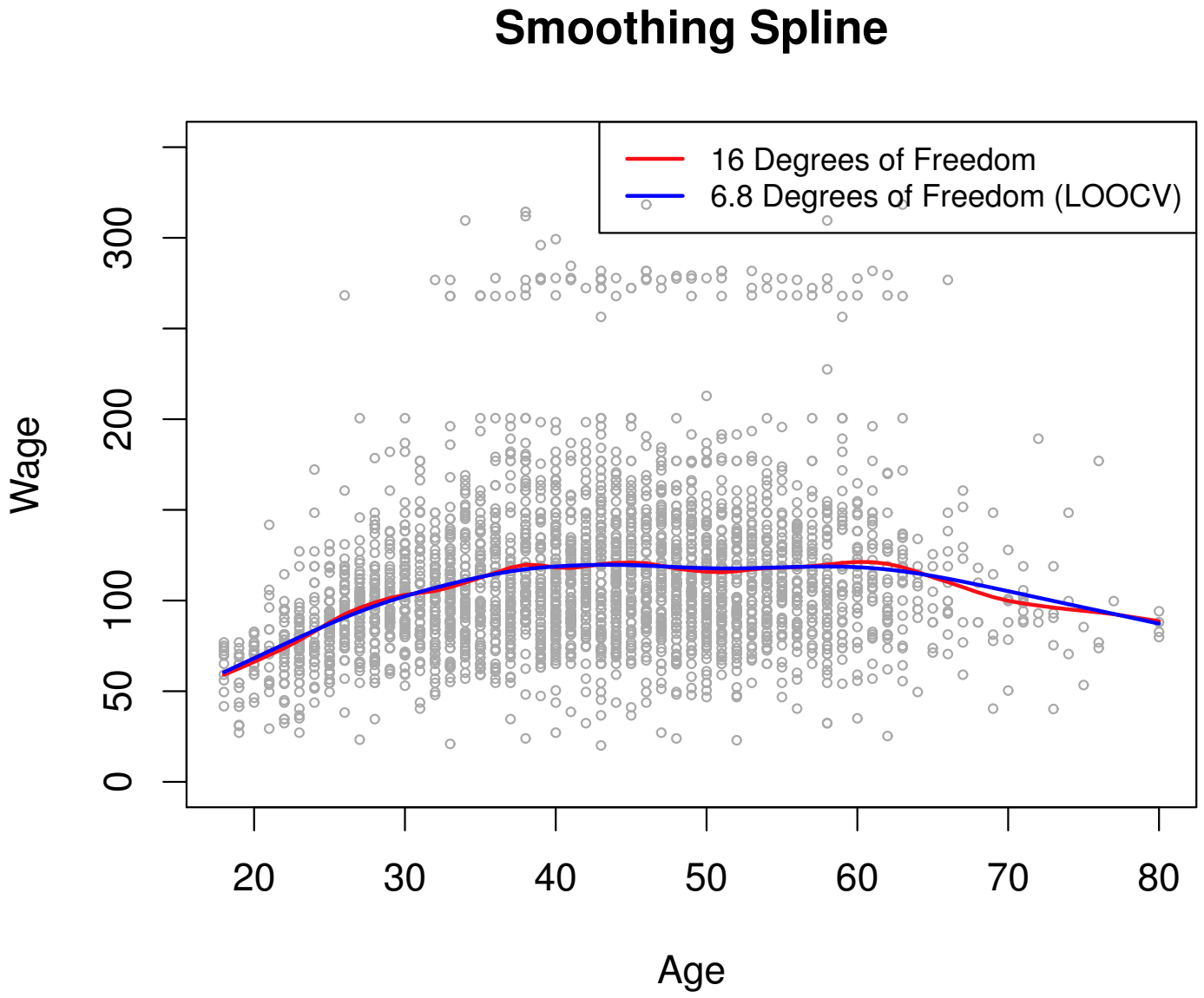


Figure: 7.8 from ISLR. We'll introduce LOOCV (leave-one-out cross-validation) in Part II of today's class

Another method people like: Local regression

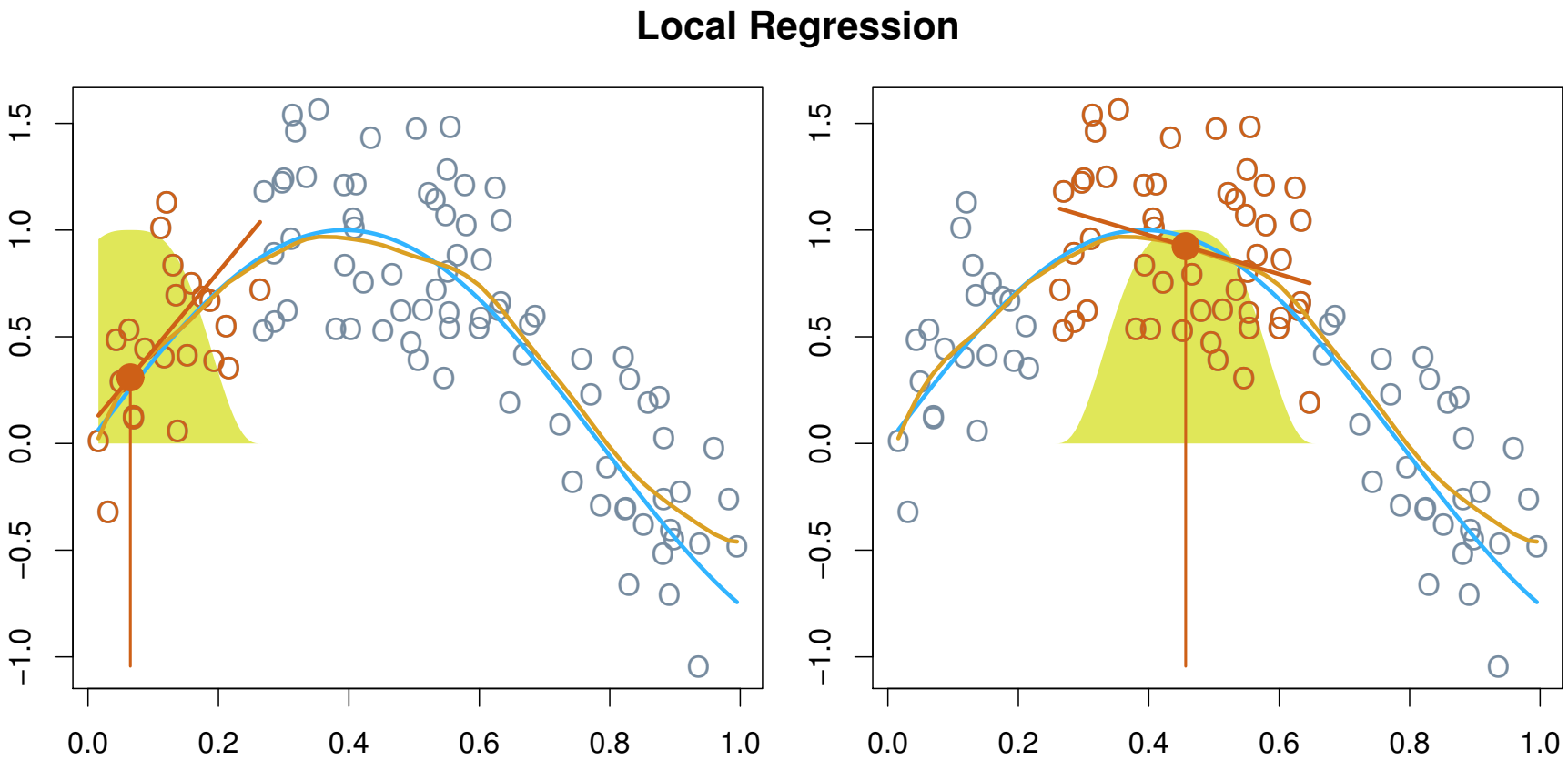
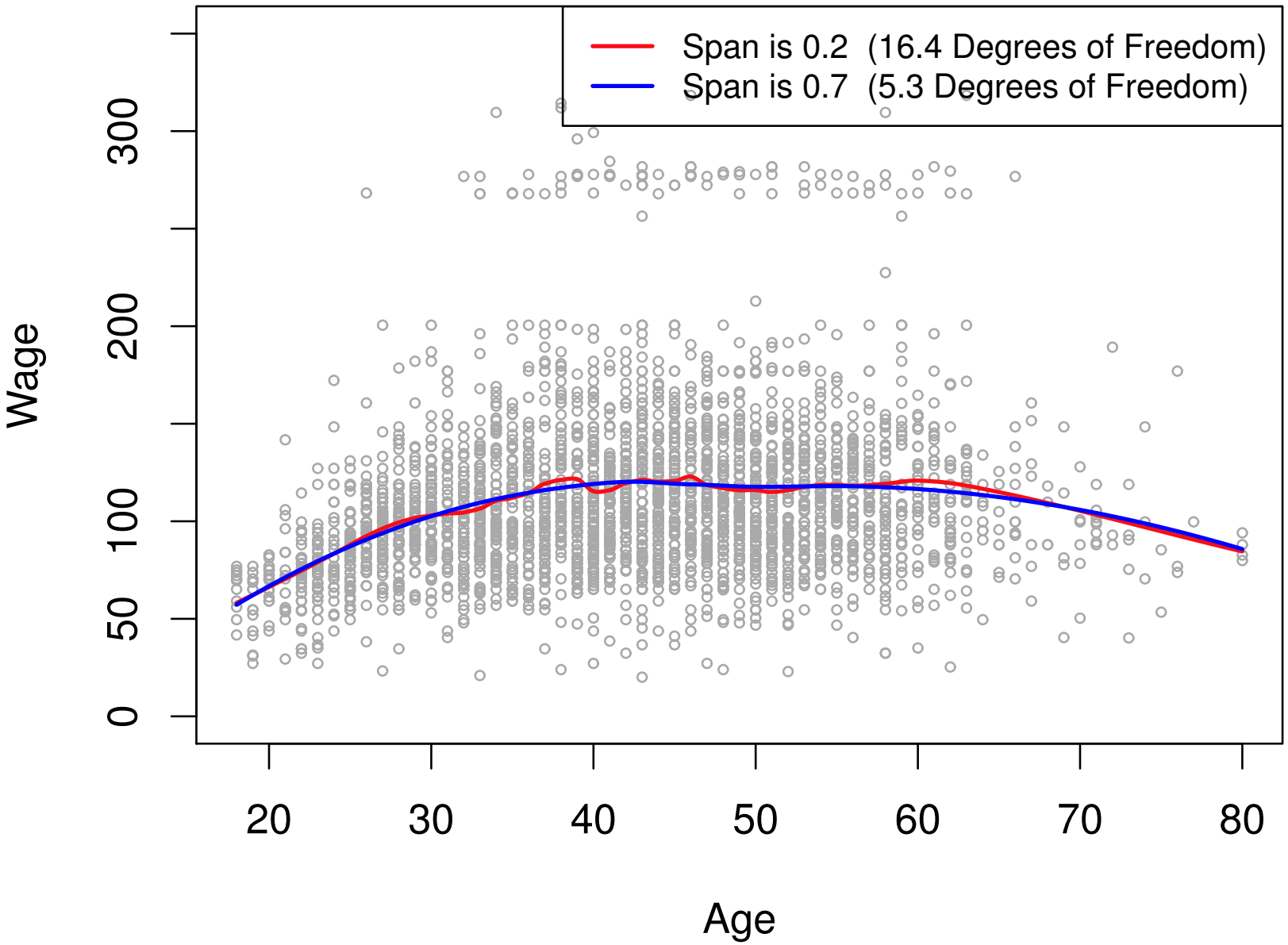


Figure: 7.9 from ISLR. Local regression (enabled as `lo(x)` and `loess(x)`)

Local Linear Regression



Putting everything together: Additive Models

- Recall the Linear Regression Model

$$Y = \beta_0 + \sum_{j=1}^{p} \beta_j X_j + \epsilon$$

- We can now extend this to the far more flexible Additive Model

$$Y = \beta_0 + \sum_{j=1}^{p} f_j(X_j) + \epsilon$$

- Each f_j can be any of the different methods we just talked about: Linear term $(\beta_j X_j)$, Polynomial, Step Function, Piecewise Polynomial, Degree-k spline, Natural cubic spline, Smoothing spline, Local linear regression fit, …
- You can mix-and-match different kinds of terms
- The `gam` and `mgcv` packages enable Additive Models in **R**

Additive Models: Boston housing data

Using the `gam`[4] library, we fit the model

```
gam(medv ~ s(lstat, 5) + lo(ptratio) +
           cut(crim, breaks = c(-Inf, 1, 10, 25, Inf)),
           data = Boston)
```

- This amounts to an additive model

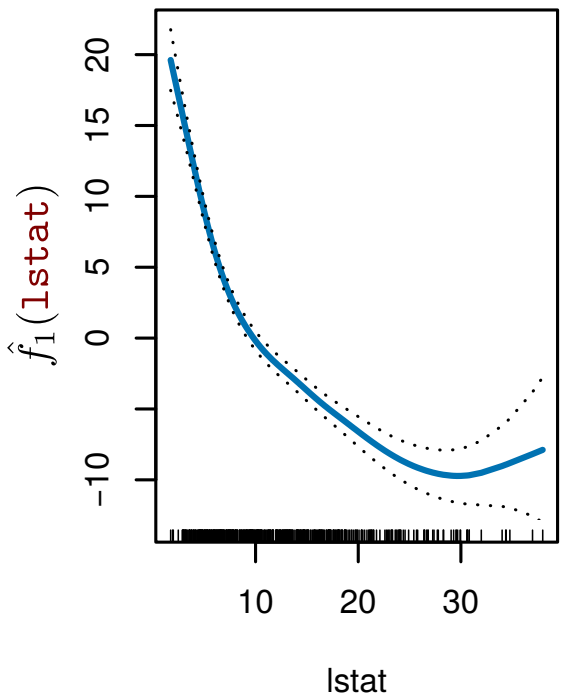
$$\texttt{medv} = f_1(\texttt{lstat}) + f_2(\texttt{ptratio}) + f_3(\texttt{crim}) + \epsilon$$

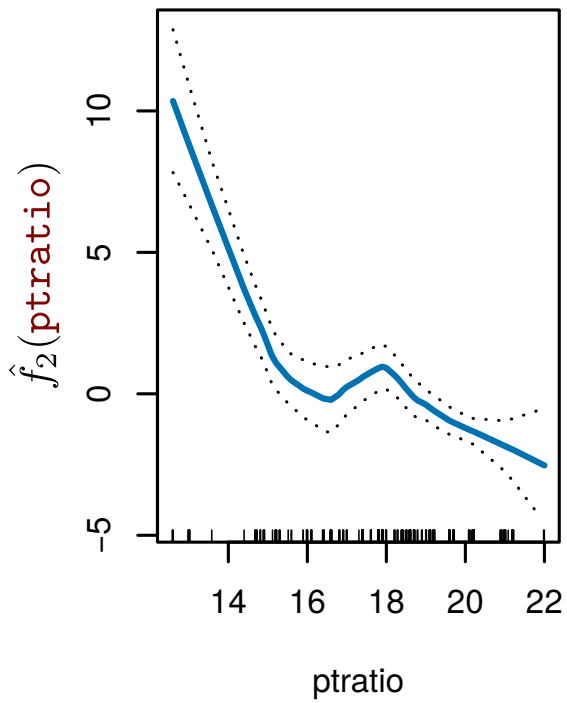
with terms:

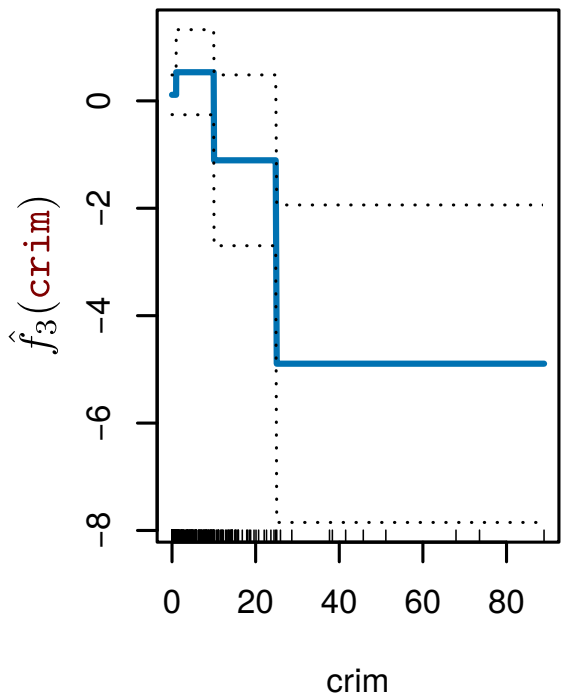
- $f_1(\texttt{lstat})$ smoothing spline with 5 df
- $f_2(\texttt{ptratio})$ local linear regression
- $f_3(\texttt{crim})$ step function with breaks at $\texttt{crim} = 1, 10, 25$

[4] You can use `lm` here instead, but `gam` has built-in plotting routines to help better visualize the model fits.

Additive Models: Boston housing data








```
gam(medv ~ s(lstat, 5) + lo(ptratio) +
           cut(crim, breaks = c(-Inf, 1, 10, 25, Inf)),
           data = Boston)
```

Summary

- Splines are a nice way of modeling *smooth* regression functions
- To increase the *flexibility* of a spline, we increase the number of knots
- Natural cubic splines allow us *retain the model complexity of a cubic spline* while adding *two extra interior knots* at the cost of restricting our model to be *linear* outside the range of the observed data
- Smoothing splines enable us to avoid the problem of knot selection altogether, and instead specify a single parameter: the desired effective degrees of freedom for the fit
- We can put everything together into an Additive Model

$$Y = \beta_0 + \sum_{j=1}^{p} f_j(X_j) + \epsilon$$

where each f_j can be any of the fits we talked about.

Introduction to Model Selection

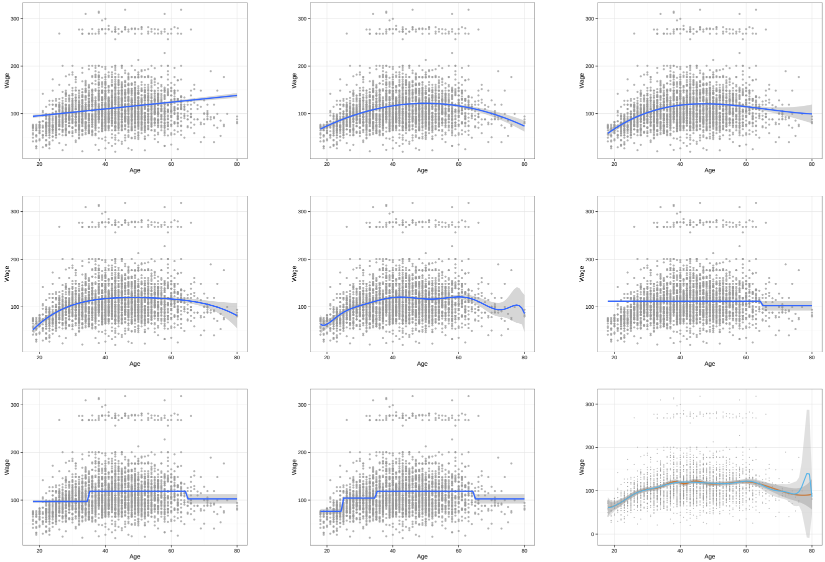
At this stage, we have a lot of questions.

- How do we choose which variables to include in a linear regression?
- How do we choose the degree k in a polynomial regression?
- How do we choose the cuts in a step function regression?
- How do we decide on how many knots to place and where to place them when fitting regression splines?
- How should we choose λ or the effective degrees of freedom for a smoothing spline?
- Which variables should we include in an additive model, and what form should we pick for each f_j term?

All of these questions are essentially asking the same thing...

How do we pick the best model?

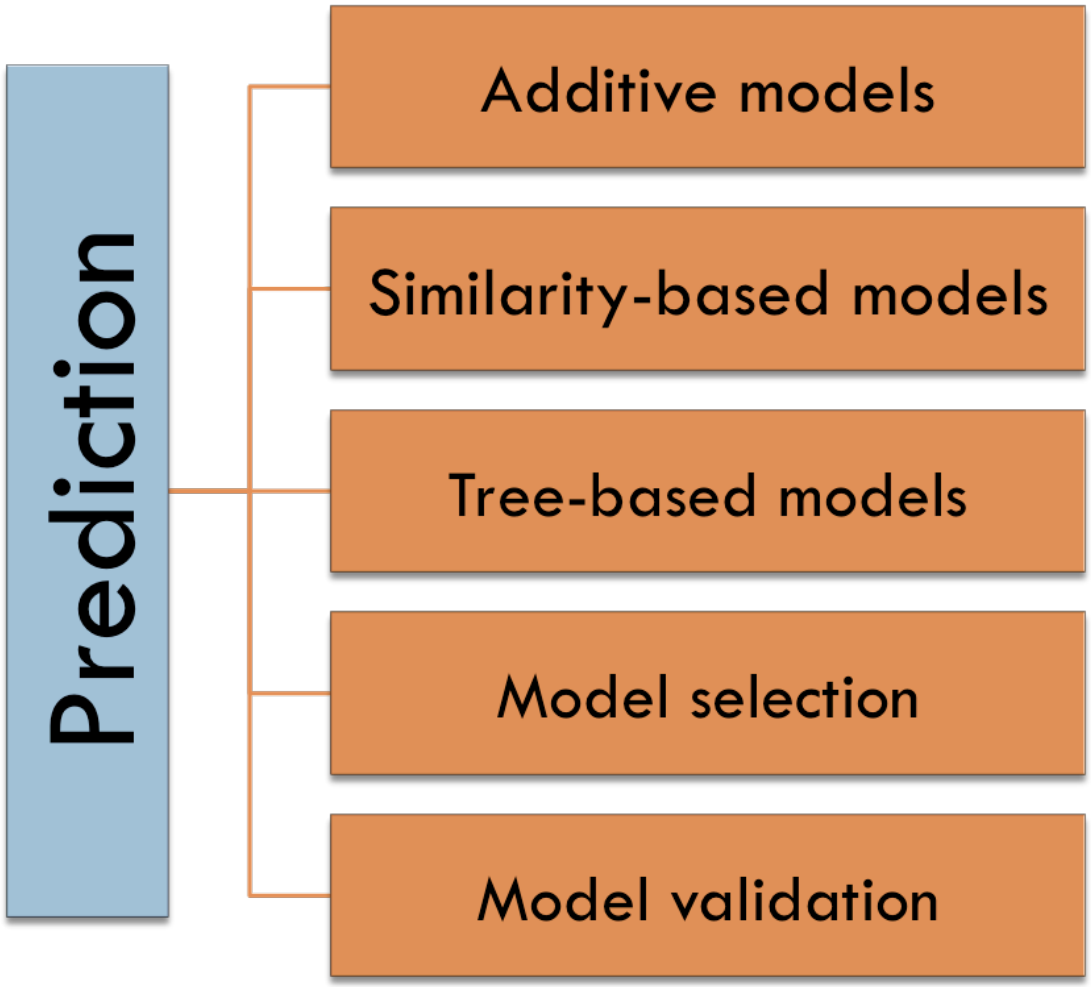
How do we pick the best **statistical** model?



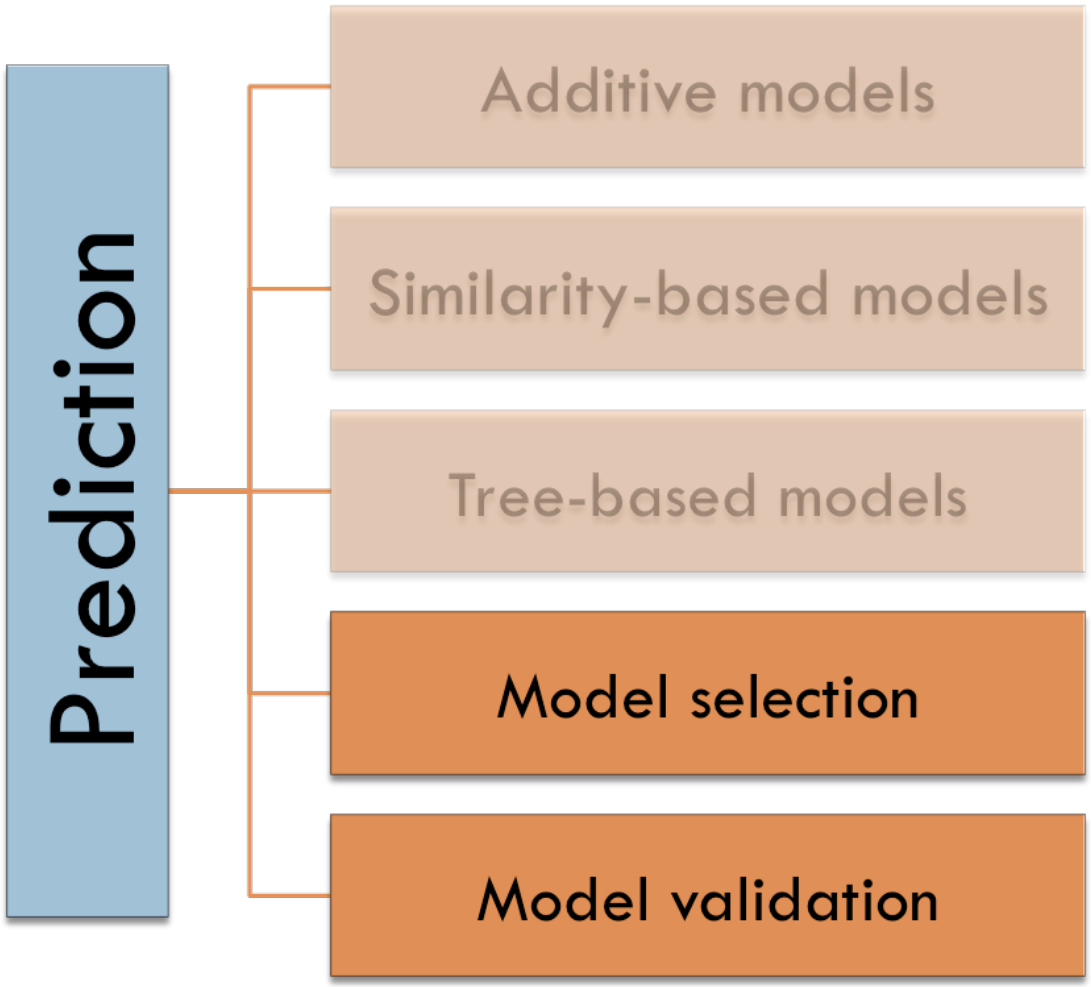
End of Part I

10 minute break

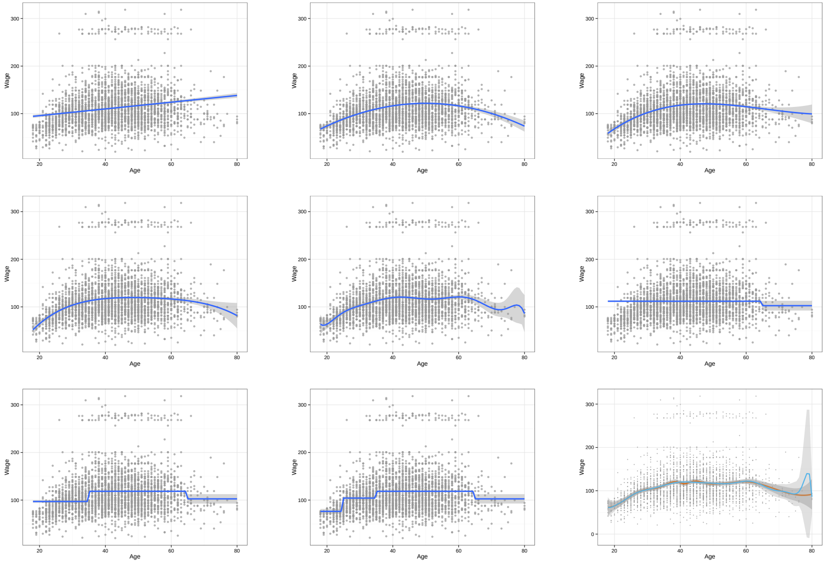
Prediction topics: Part II



Prediction topics: Part II



How do we pick the best **statistical** model?



Resampling methods

- Part II of today's lecture covers several topics that fall into the category of Resampling methods
- These are approaches for using a single observed data set to answer questions such as:
  - Which model generalizes best to *unseen data*?
  - What is the prediction error of my model?
  - What is the *uncertainty* of my estimate?
  - How can I form a *confidence interval* for a complex parameter?

Agenda for Part II

- **Review: Central Themes**
- **Test error vs. Training error**
- **Resampling methods**
  - Validation set approach (Train/Test split)
  - Cross-validation
- **Stepwise/Criteria-based methods (Next class)**
  - Best subset selection
  - Stepwise model selection
  - AIC, BIC

How should we think about model selection?

Let's remind ourselves of the first Central Theme of this class.

1. **Generalizability:** We want to construct models that generalize well to unseen data

- i.e., We want to:
  1. Add variables/flexibility as long as doing so helps capture meaningful trends in the data (avoid *underfitting*)
  2. Ignore meaningless random fluctuations in the day (avoid *overfitting*)

How should we think about model selection?

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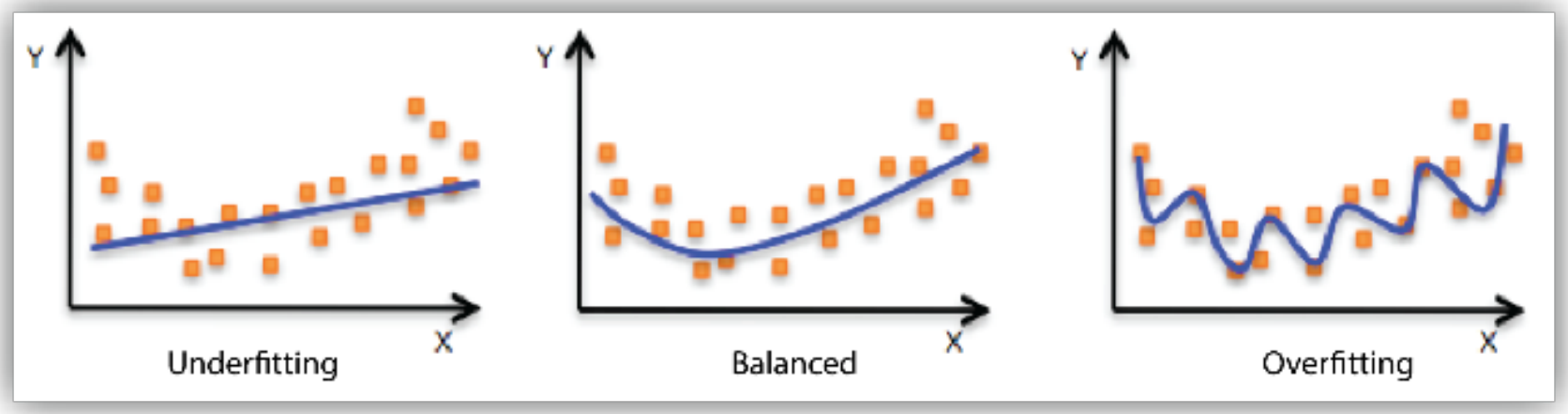


Assessing Model Accuracy

- Suppose we fit a model $\hat{f}(x)$ to some training data: $\text{Train} = \{x_i, y_i\}_{i=1}^n$.
- We want to assess how well $\hat{f}$ performs
- Can compute: Average squared prediction error over Train

$$\text{MSE}_{\text{Train}} = \underset{i \in \text{Train}}{\text{Ave}} \left[(y_i - \hat{f}(x_i))^2 \right]$$

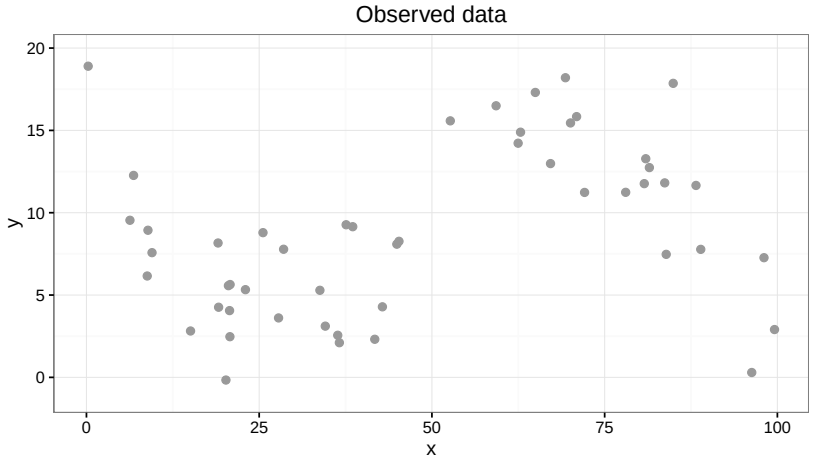
- But this may push us towards more *overfit* models.
- Instead, we should compute it using fresh test data: $\text{Test} = \{x_i, y_i\}_{i=1}^m$:

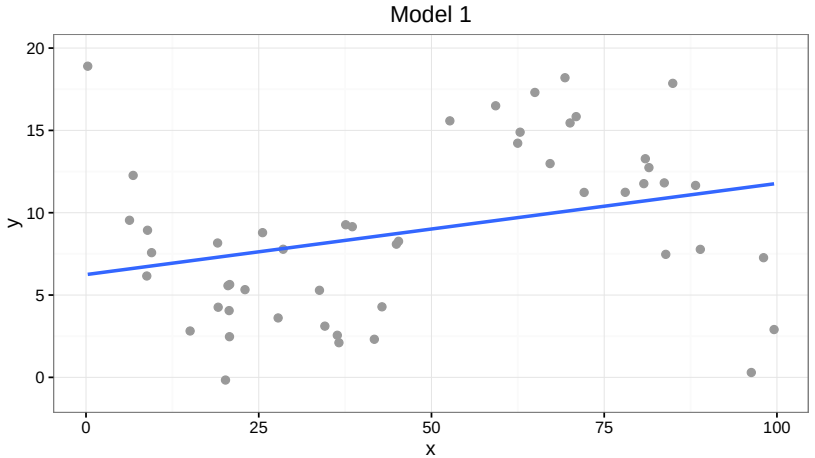
$$\text{MSE}_{\text{Test}} = \underset{i \in \text{Test}}{\text{Ave}} \left[(y_i - \hat{f}(x_i))^2 \right]$$

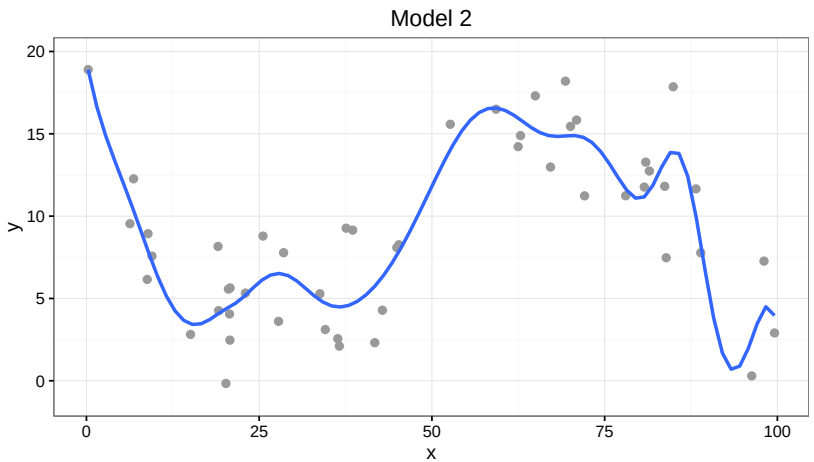
- This would tell us if $\hat{f}$ generalizes well to *new* data

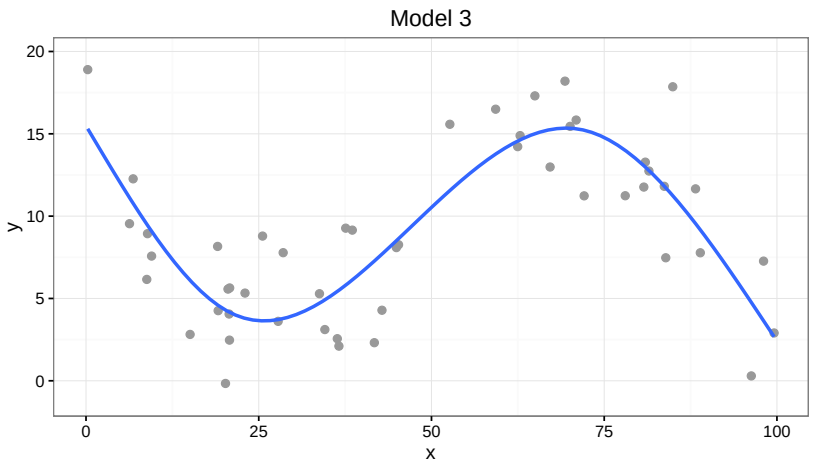
Assessing Model Accuracy: Training Error vs. Testing Error

Here are three different models fit to the same small Train data set.
Which of these three is the *best model*?

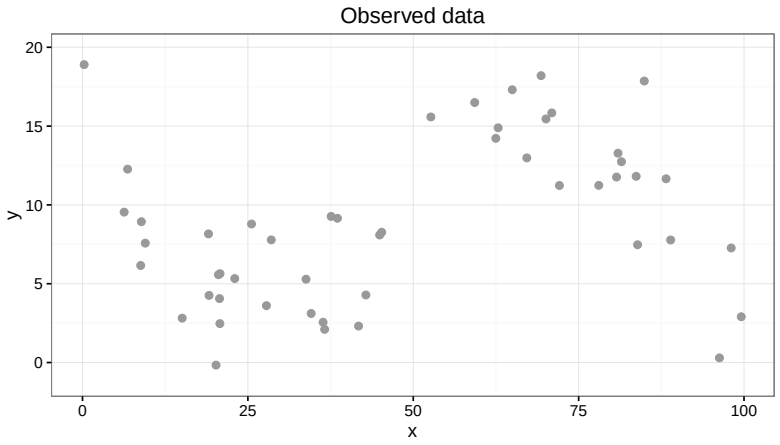


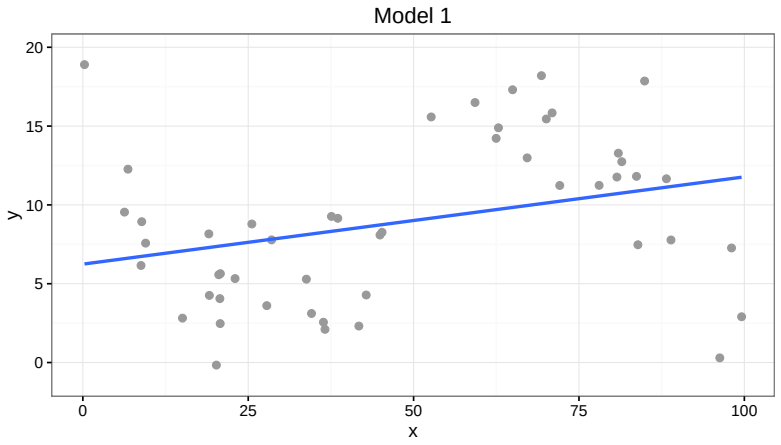


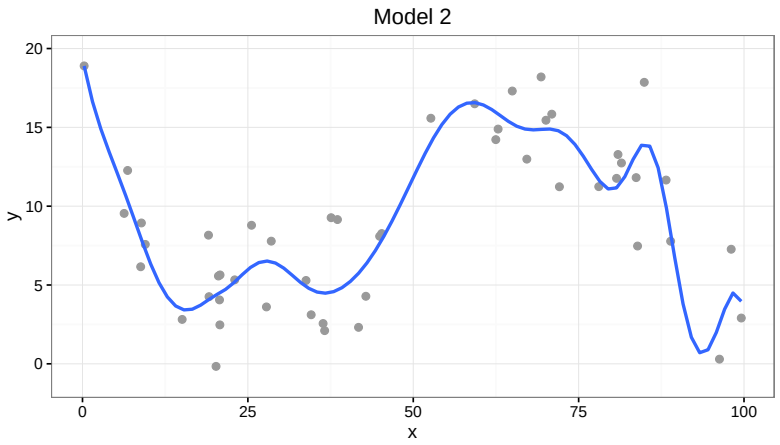


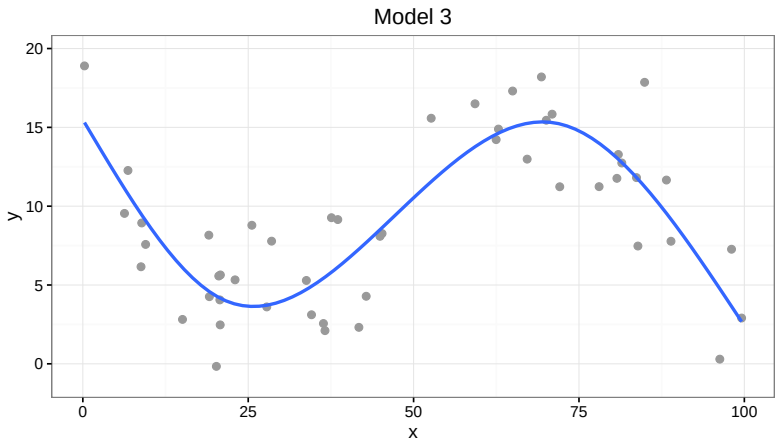


Assessing Model Accuracy: Training Error vs. Testing Error





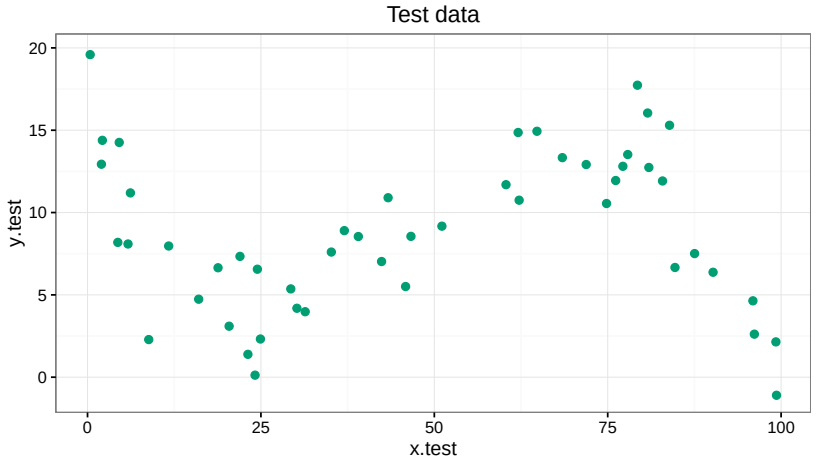


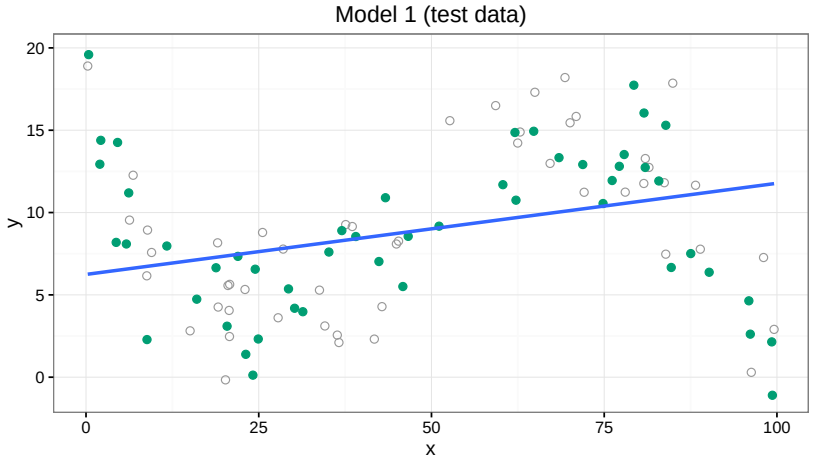


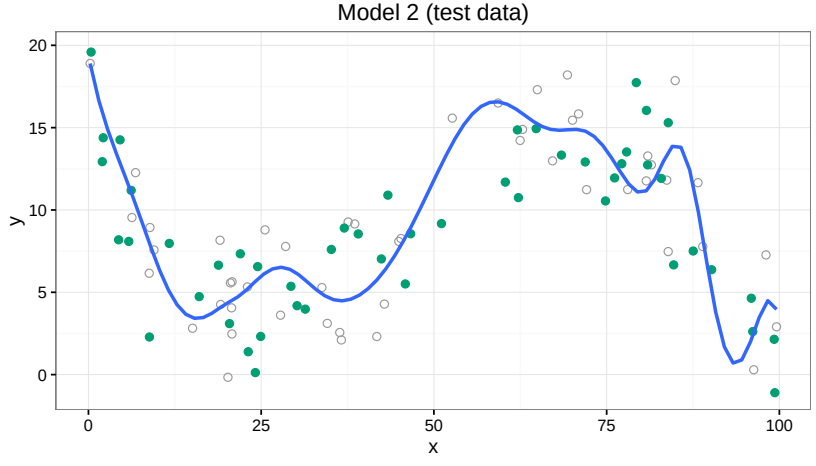
Model	1	2	3
$\text{MSE}_{\text{Train}} = \text{RSS}/n$	23.2	5.2	7.5

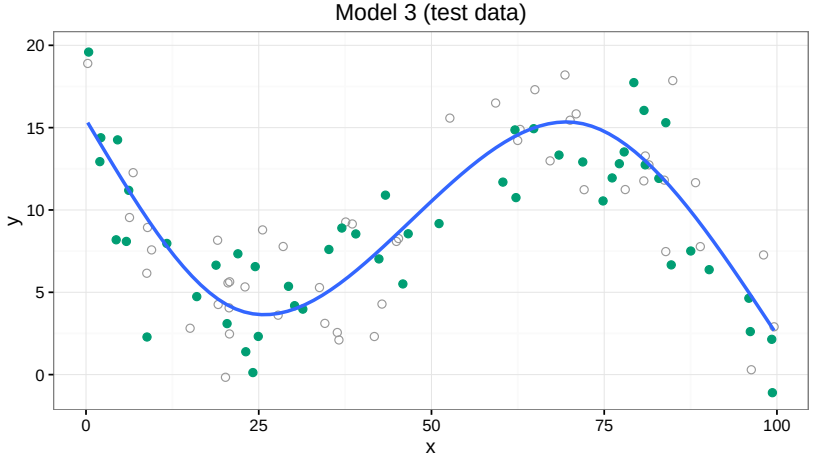
Assessing Model Accuracy: Training Error vs. Testing Error

Here are some new observations, which form our Test data. How well do our models fit the *test data*?





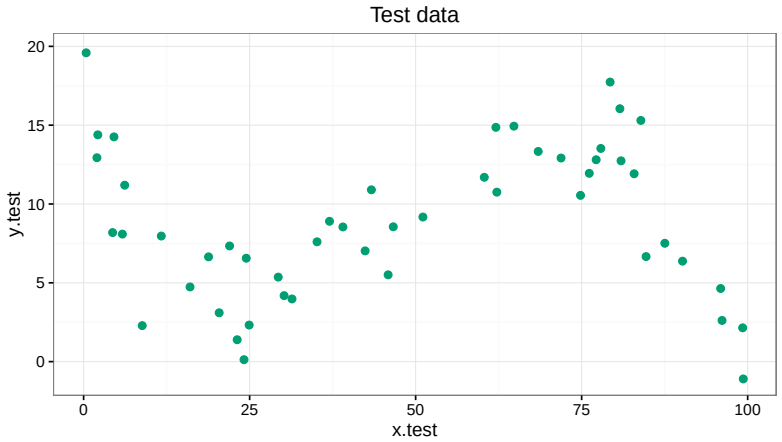


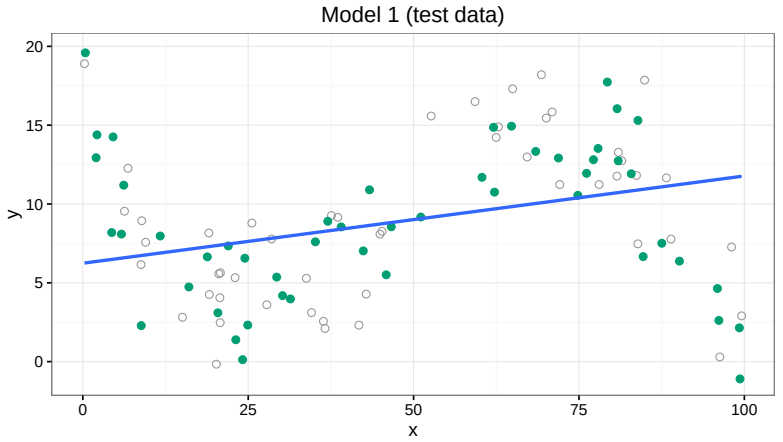


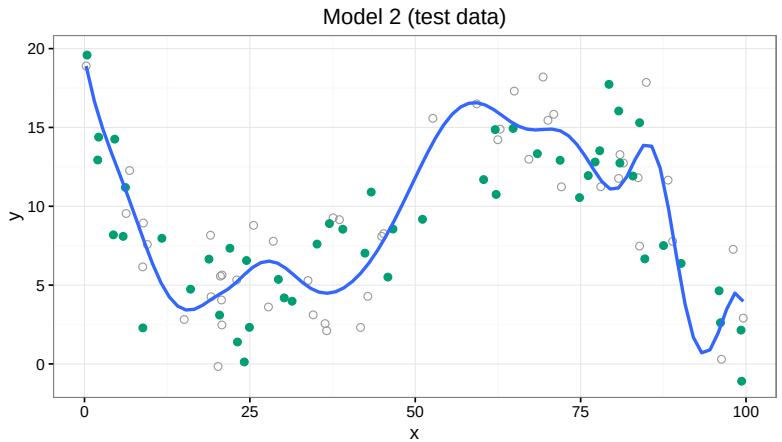
Solid green points: Test data

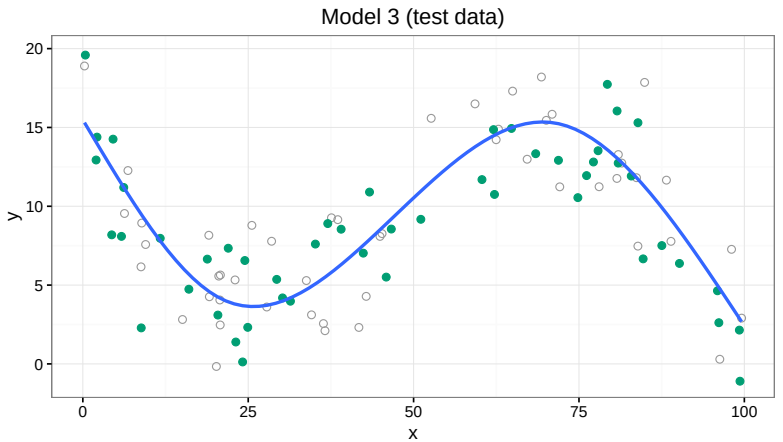
Open grey circles: Train data

Assessing Model Accuracy: Training Error vs. Testing Error









Model	1	2	3
$\text{MSE}_{\text{Train}}$	23.2	5.2	7.5
MSE_{Test}	24.6	10.3	7.0

Assessing Model Accuracy

- As we increase the flexibility of our model, our training set error always decreases
- The same is **not** true for test set error
- The test set error will *decrease* as we add flexibility that helps to capture useful trends
- As we add *too much* flexibility, the test set error will begin to *increase* due to model overfitting

How well could we possibly do?

- There is a limit on how well we can do on any given prediction task
- Even if we knew the true regression function $f(x) = \mathbb{E}(Y \mid X = x)$, we would still have error:

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

- $\epsilon = Y - f(x)$ is the irreducible error.
- Even if we knew $f(x)$, we would still make errors in prediction: Because at each value of x, there's typically a distribution of possible Y values
- Our average prediction error will always be at least $\mathrm{Var}(\epsilon)$

Bias-Variance trade-off in prediction

Let's remind ourselves of the second Central Theme of the class:

2. **Bias-Variance trade-off:** To minimize prediction error, we need to find the right balance between the *bias* and *variance* of our predictor $\hat{f}$

- Suppose we some Train data, which we use to build a predictor $\hat{f}$
- For any predictor $\hat{f}$, one can decompose the the *expected test MSE*[5] at a new data point x_0 as:

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

[5] For more details, read §2.2.2 of ISL

Bias-Variance trade-off in prediction

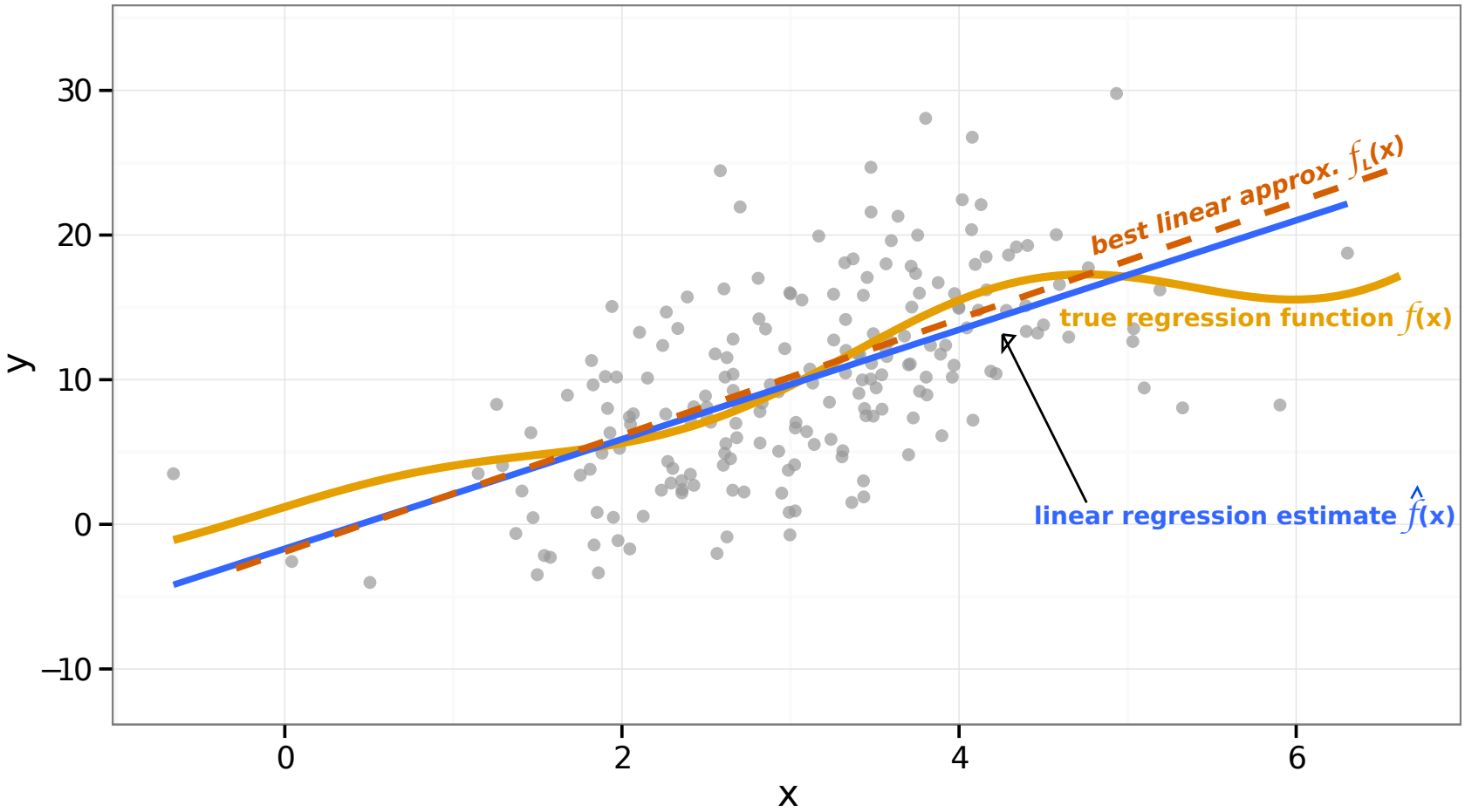
Let's understand what this equation is saying

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

- $\mathbb{E}\left[(y_0 - \hat{f}(x_0))^2\right]$ is the expected test MSE:
  - It's the average test MSE we would get if we repeatedly constructed $\hat{f}$ using a large number of random training sets, and tested each at x_0, with random realizations of y_0.
- $\mathrm{Var}(\hat{f}(x_0))$ is the variance of $\hat{f}$ at x_0.
  - It's the variability of $\hat{f}(x_0)$ around $\mathbb{E}\,\hat{f}(x_0)$
- $\mathrm{Bias}(\hat{f}(x_0))$ is the bias of $\hat{f}$ at x_0

$$\begin{aligned}\mathrm{Bias}(\hat{f}(x_0)) &= \mathbb{E}\,\hat{f}(x_0) - \mathbb{E}\,(Y \mid X = x_0) \\ &= \mathbb{E}\,\hat{f}(x_0) - f(x_0)\end{aligned}$$

- $\mathrm{Var}(\epsilon)$ is the irreducible error



Variance measures how much $\hat{f}(x_0)$ varies around $f_L(x_0)$

Bias measures how far $f_L(x_0)$ is from the true regression function $f(x_0)$

Bias-Variance trade-off in prediction

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

- This quantity is the *expected test MSE* at a particular value x_0
- The overall test MSE can be calculated by further averaging this quantity over all possible values of x_0 in the test set

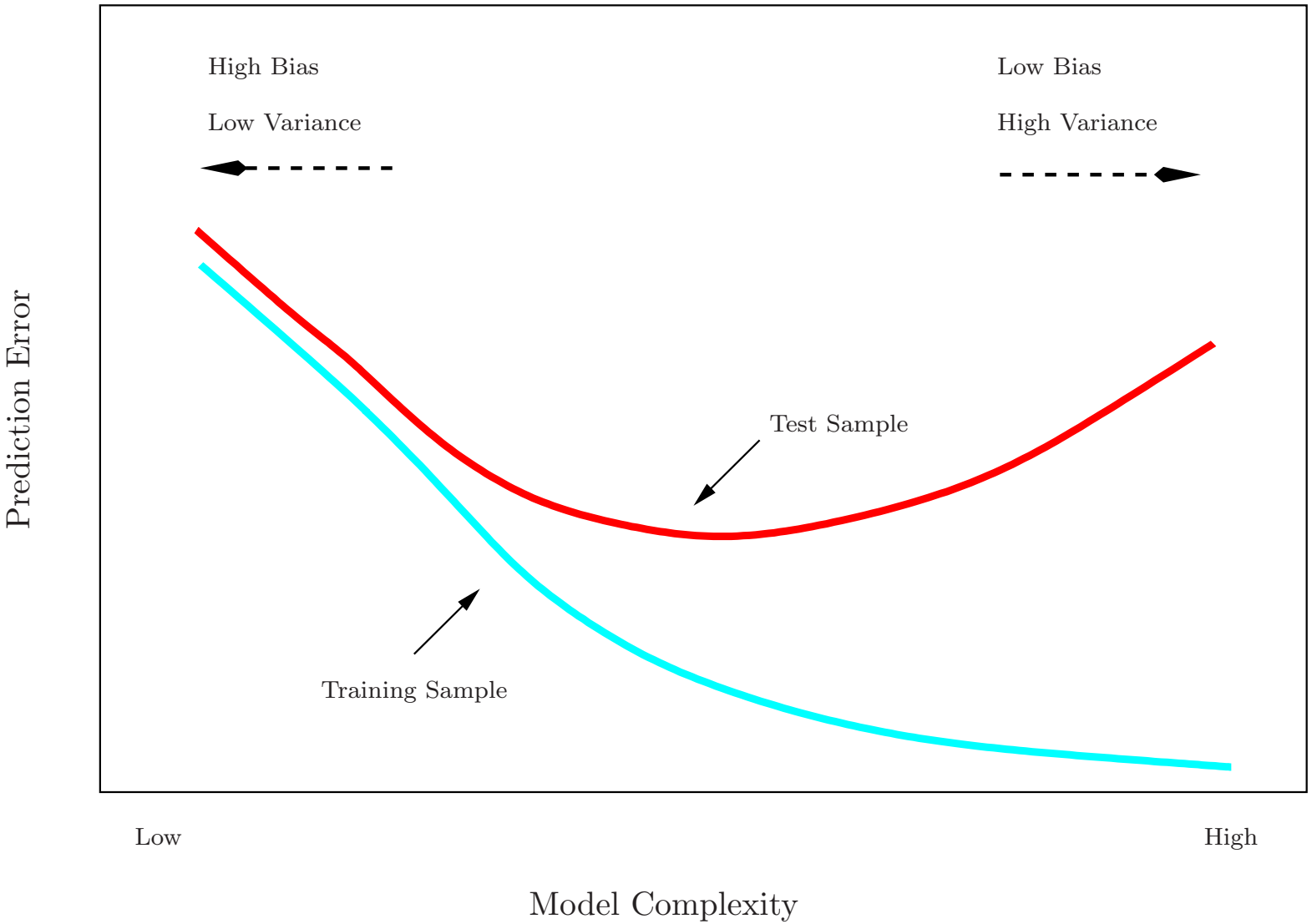
Bias-Variance trade-off in prediction

Let's think about this equation in practical terms

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

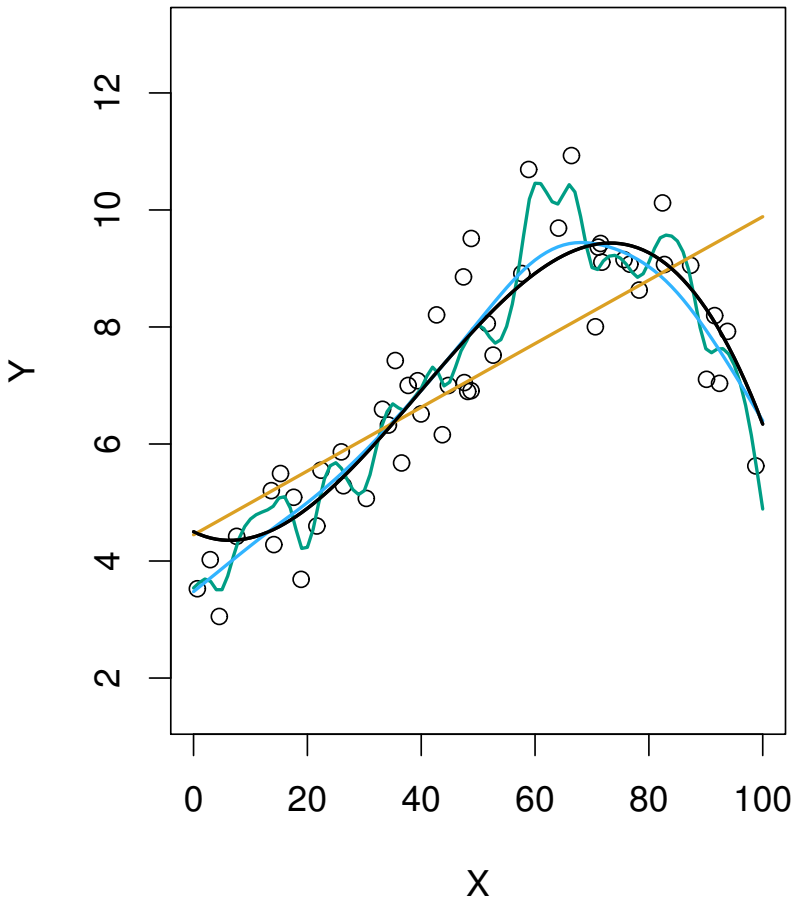
- Variance refers to how much $\hat{f}$ would change if we estimated it using a different random set of training data
  - Training data is random, different Training data will result in different $\hat{f}$
  - Ideally, $\hat{f}$ should not change tremendously between different Training sets
  - If small changes in Training data change $\hat{f}$ by a lot, then $\hat{f}$ would have High Variance
- Bias refers to error introduced by modeling a complex real-world problem by a simpler statistical model
  - E.g., Linear regression assumes a linear relationship between Y and the inputs $X_1, \ldots, X_p$. This is almost always an over-simplification
  - If the true f is very complex and $\hat{f}$ is too inflexible, $\hat{f}$ will have High Bias

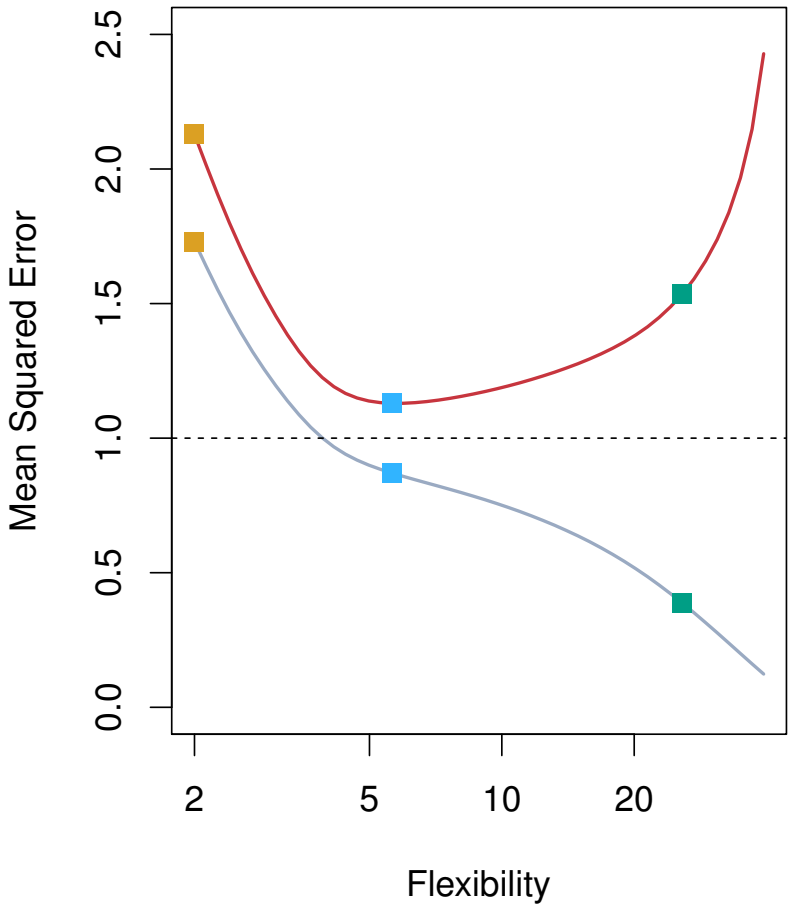
Key Picture


High Bias
Low Variance
Low Bias
High Variance
Test Sample
Training Sample
Prediction Error
Low
High
Model Complexity

Training Error vs Test Error: Example 1

Dashed line on MSE plot shows the irreducible error $\mathrm{Var}(\epsilon)$



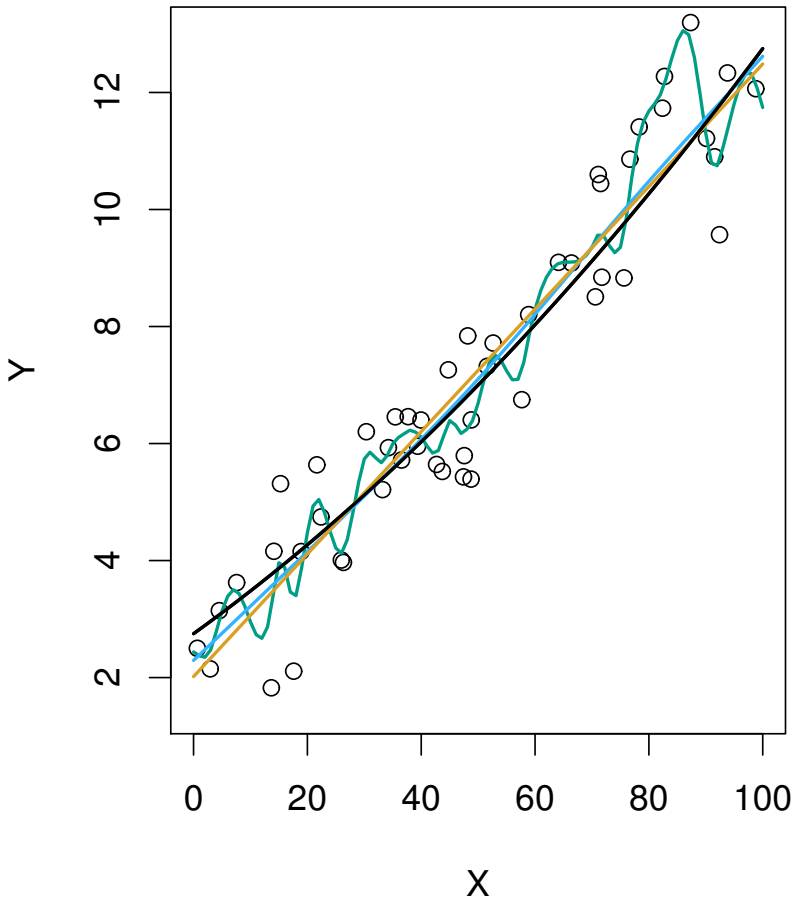


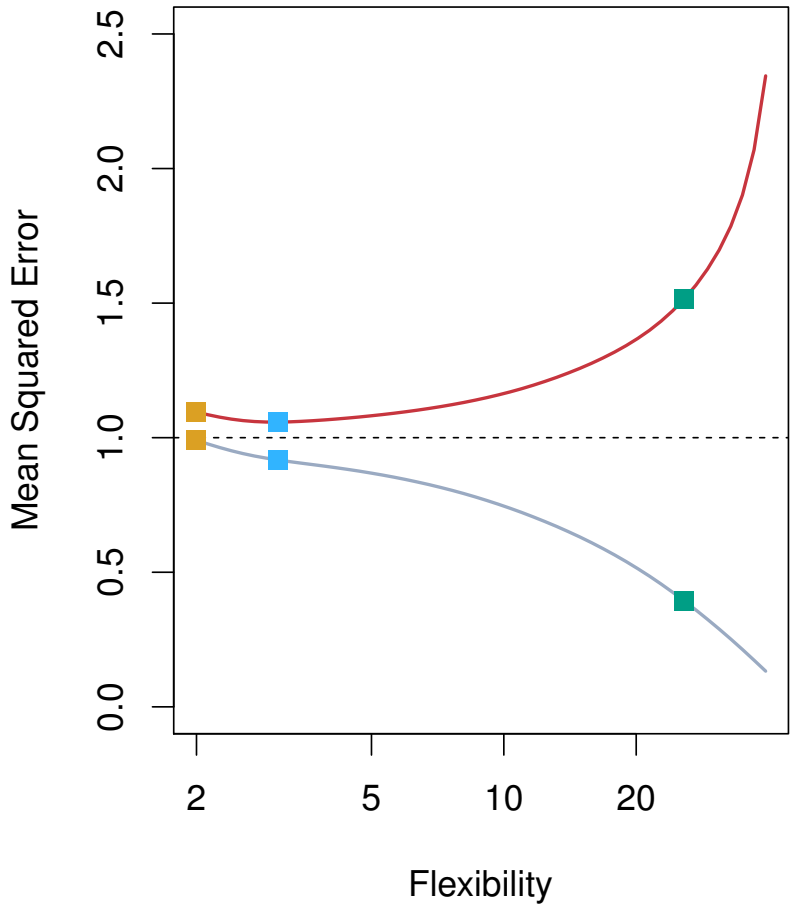
Left: Models fit to training data. Black curve is the truth.

Right: $\mathrm{MSE}_{\mathrm{Train}}$ in grey, $\mathrm{MSE}_{\mathrm{Test}}$ in red

Training Error vs Test Error: Example 2

Dashed line on MSE plot shows the irreducible error $\mathrm{Var}(\epsilon)$

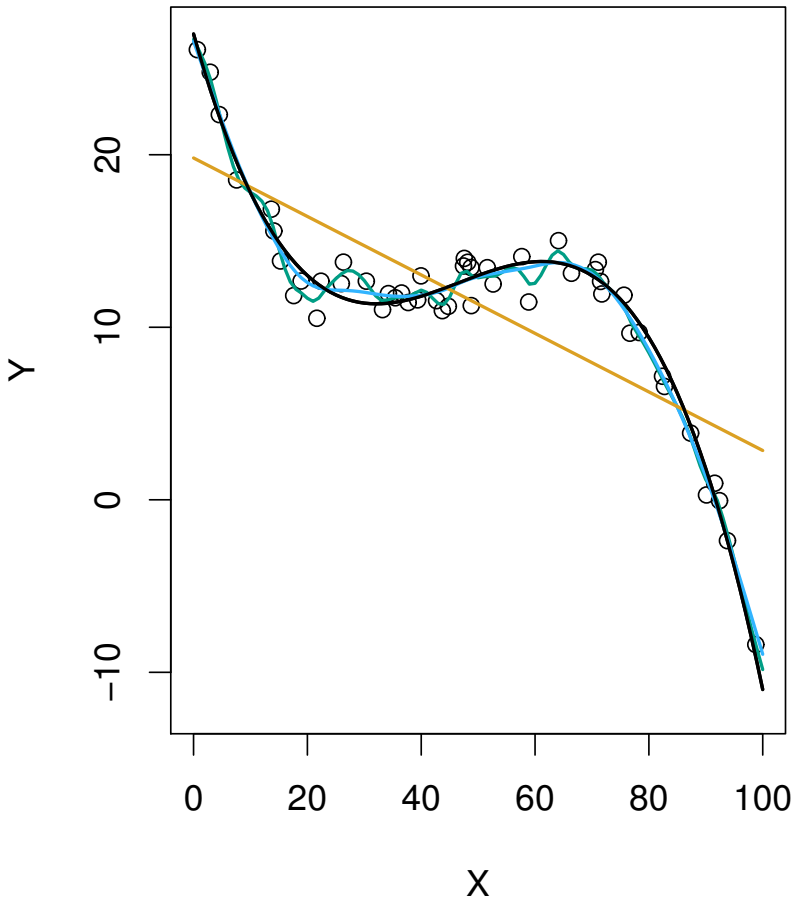


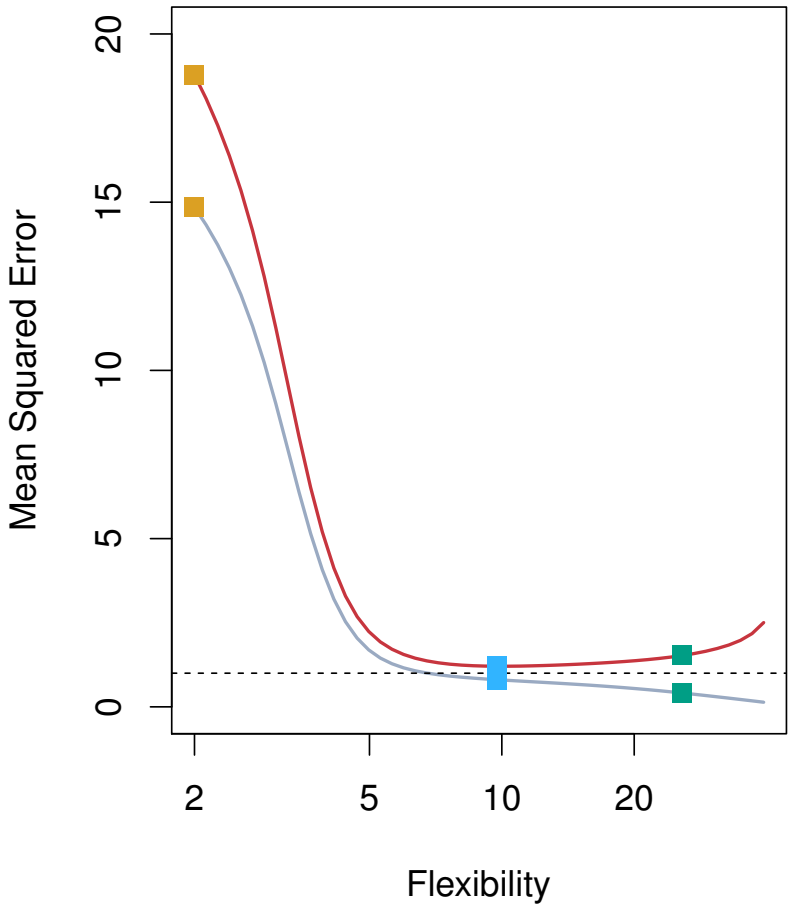


Truth (black curve) is simpler/smoother (nearly linear), so the smoother fit and linear model both perform really well.

Training Error vs Test Error: Example 3

Dashed line on MSE plot shows the irreducible error $\mathrm{Var}(\epsilon)$

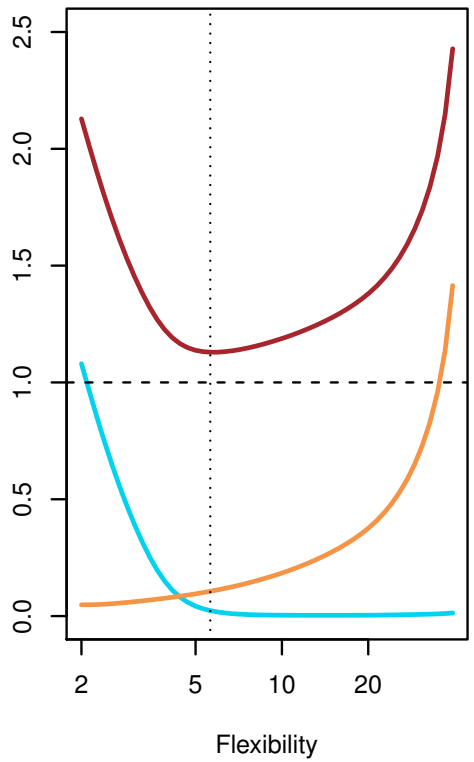




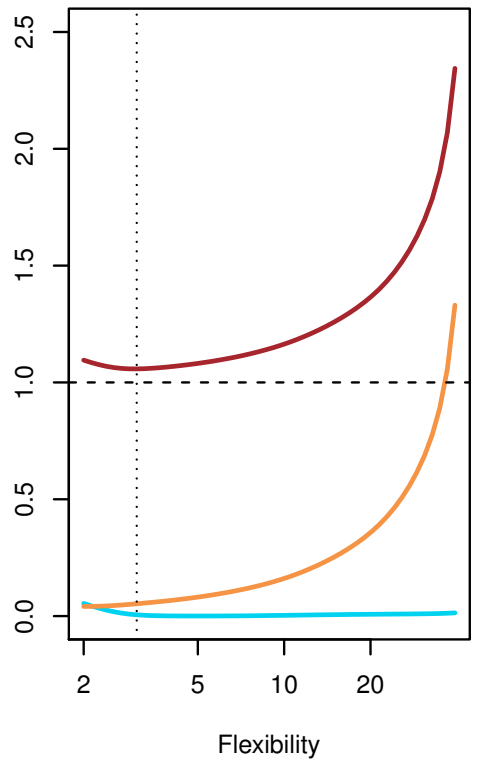
Truth is wiggly, but noise level is very low. The more flexible fits perform the best.

Bias-Variance Trade-off for the three examples

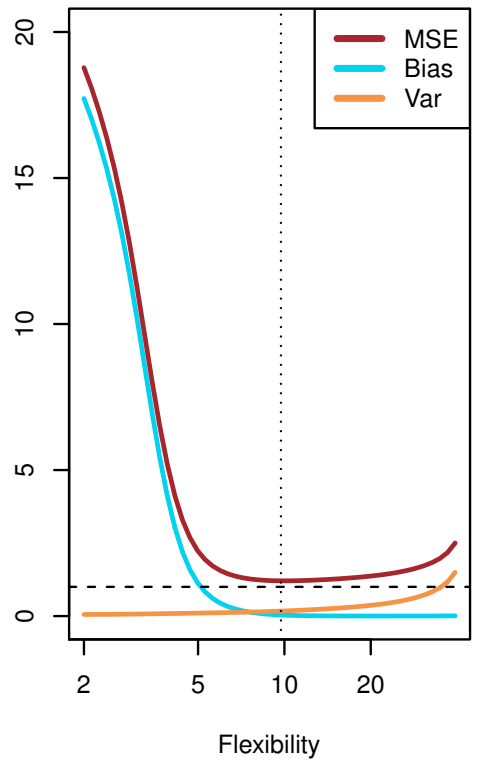
Dashed lines show the irreducible error $\mathrm{Var}(\epsilon)$



Example 1



Example 2



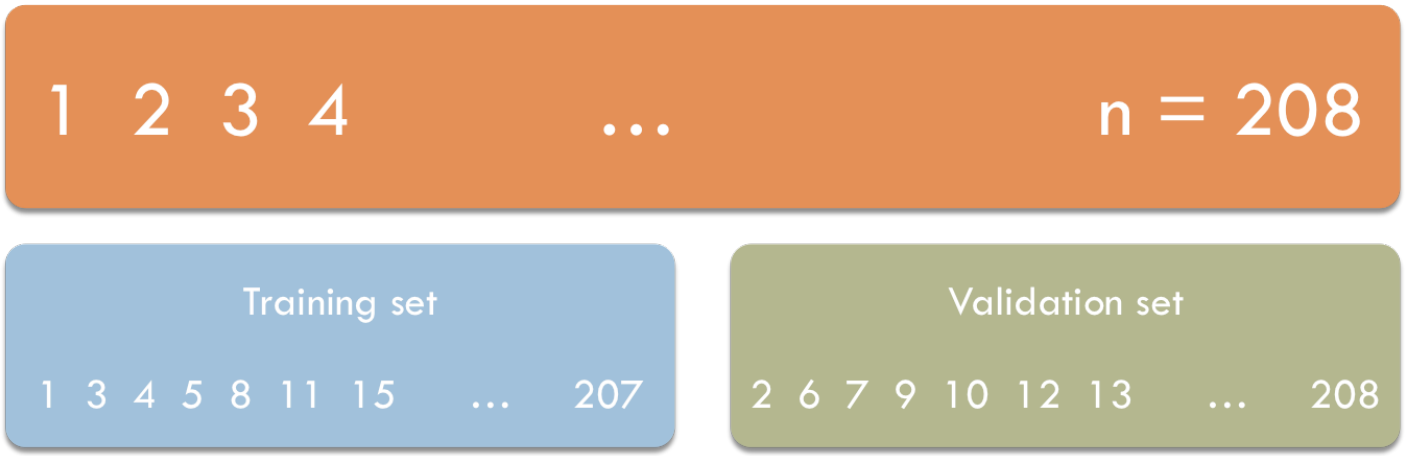
Example 3

How do we estimate the Test Error?

- In reality, we only get one set of data to use for model fitting, model selection, and model assessment
- We will now discuss two methods for estimating Test Error:
  - Validation set approach
  - Cross-validation
- We will explain why Cross-validation is generally the best approach

Validation set approach

1. Randomly divide the available data into two parts: a Training set and a Validation or Hold-out set



2. Construct $\hat{f}$ by fitting your model on the Training set
3. Use $\hat{f}$ to predict responses for all the points in the Validation set, and calculate the resulting MSE
4. Pick the simplest model that has among the *lowest* MSE on the Validation set

Example: Automobile data

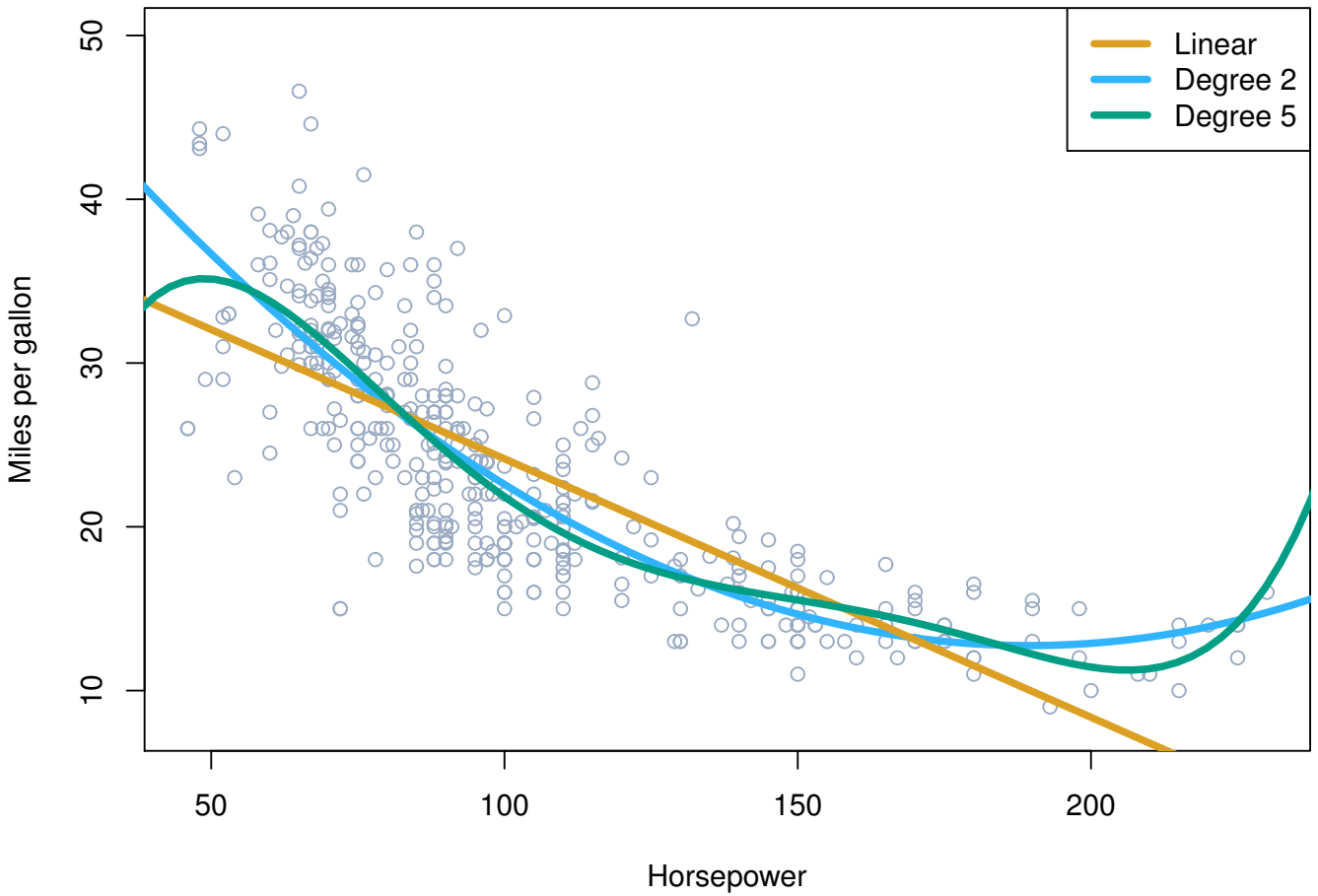


Figure: 3.8 from ISL. We want to figure out what degree polynomial we want to use to model the relationship between $Y =$ `Miles per gallon` and $X_1 =$ `Horsepower`

Example: Automobile data

- Want to figure out what degree polynomial to use
- Randomly split the 392 observations into two sets of 196 data points. Train on the *first*, calculate errors on the *second*.

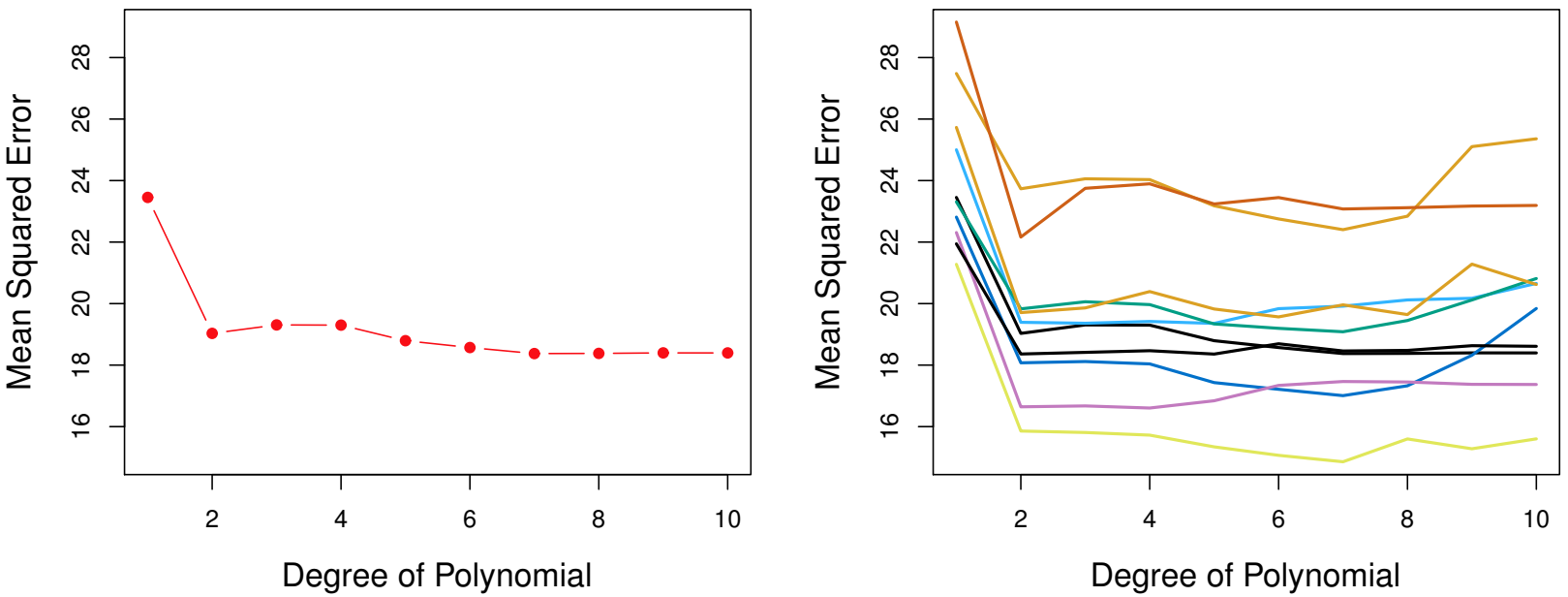


Figure 5.2 from ISL. Left panel shows MSE for a single split. Right panel shows MSE curves for 10 randomly chosen splits.

Example: Automobile data

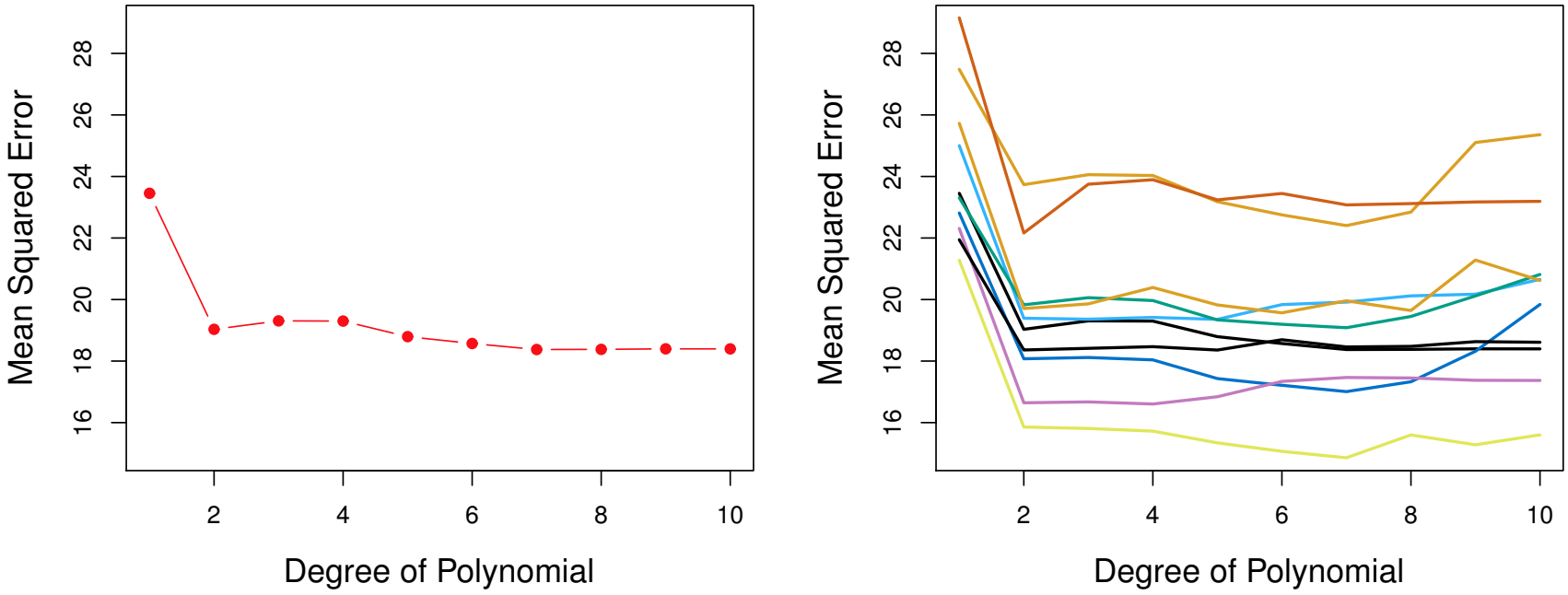
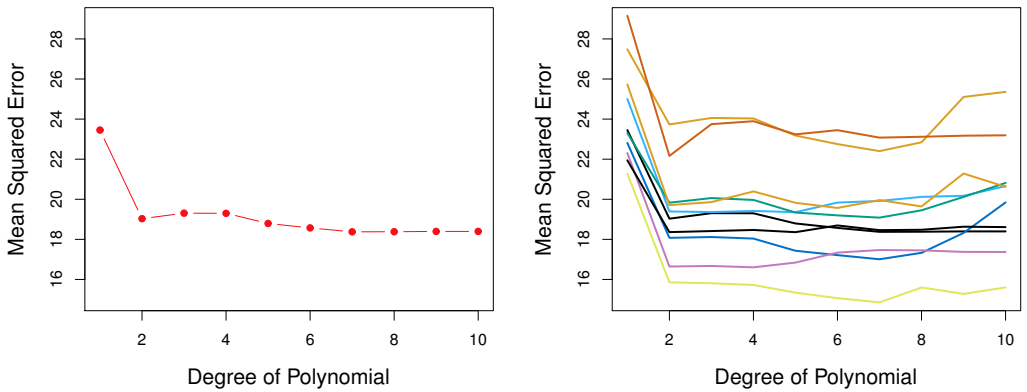


Figure 5.2 from ISL. Left panel shows MSE for a single split. Right panel shows MSE curves for 10 randomly chosen splits.

- All splits agree that quadratic is much better than *linear*
- Degree > 2 fits don't seem to perform considerably better than quadratic

Problems with the Validation set approach



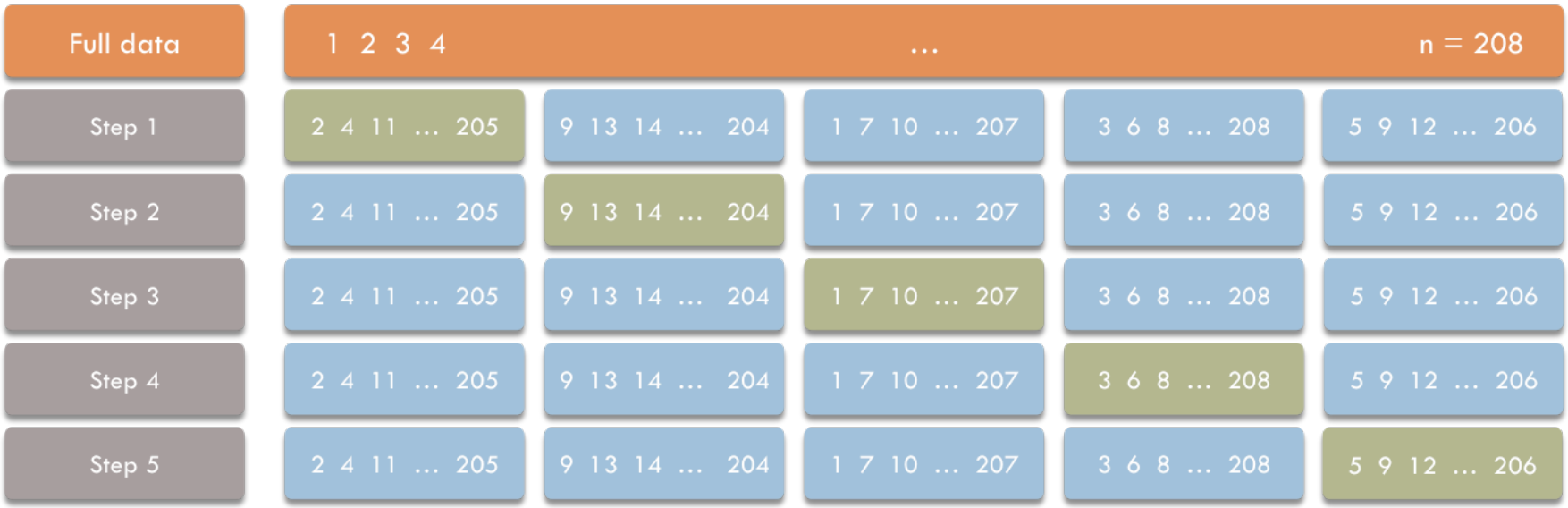
1. As observed in the right-hand panel, the estimates of Test Error are highly variable. Estimates depend a lot on the randomly chosen split.
2. Only a subset of the data (the ones randomized to the Training set) are used to fit the model.
   - Models tend to perform worse when trained on fewer observations
   - The *Validation set error* tends to overestimate the *Test Error* for the model trained on the entire data set

Cross-validation is a refinement of the Validation set approach that addresses these two issues.

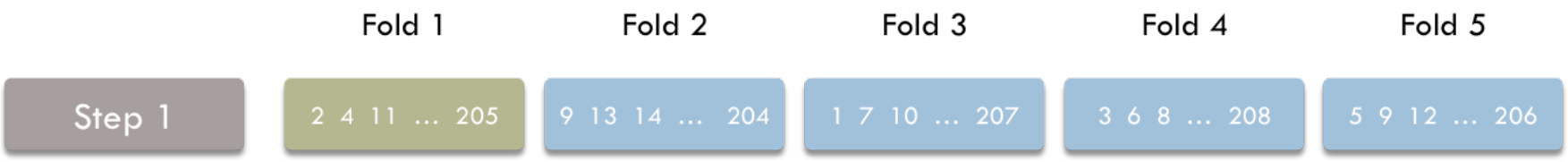
K-fold Cross-validation (CV)

- The most widely used approach for estimating Test Error
- Error estimates can be used to select the best model, and also reflect the test error of the final chosen model
- Main idea: K-fold Cross-validation
  1. Randomly split the data into K equal-sized parts ("folds")
  2. Give each part the chance to be the Validation set, treating the other $K-1$ parts (combined) as the Training set
  3. Average the test error over all of the folds
  4. Pick the simplest model among those with the lowest CV-error
  5. Final model: Refit model on the entire data set.
- Most common choices of K: 5, 10, n
  - The case $K = n$ is also known as Leave-one-out Cross-validation (LOOCV)

The Picture for 5-fold Cross-validation



The Picture for 5-fold Cross-validation



1. Use Folds 2, 3, 4, 5 as a Train set to construct $\hat{f}$

2. Use Fold 1 as Test set to calculate error:

$$\text{MSE}_1 = \sum_{i \in \text{Fold 1}} (y_i - \hat{f}(x_i))^2$$

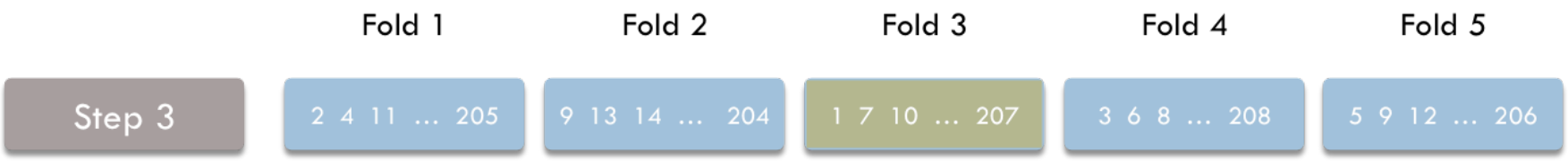
The Picture for 5-fold Cross-validation

1. Use Folds 1, 3, 4, 5 as a Train set to construct $\hat{f}$

2. Use Fold 2 as Test set to calculate error:

$$\mathrm{MSE}_2 = \sum_{i \in \text{Fold 2}} (y_i - \hat{f}(x_i))^2$$

The Picture for 5-fold Cross-validation



1. Use Folds 1, 2, 4, 5 as a Train set to construct $\hat{f}$

2. Use Fold 3 as Test set to calculate error:

$$\text{MSE}_3 = \sum_{i \in \text{Fold 3}} (y_i - \hat{f}(x_i))^2$$

The Picture for 5-fold Cross-validation

1. Use Folds 1, 2, 3, 5 as a Train set to construct $\hat{f}$

2. Use Fold 4 as Test set to calculate error:

$$\mathrm{MSE}_4 = \sum_{i \in \text{Fold } 4} (y_i - \hat{f}(x_i))^2$$

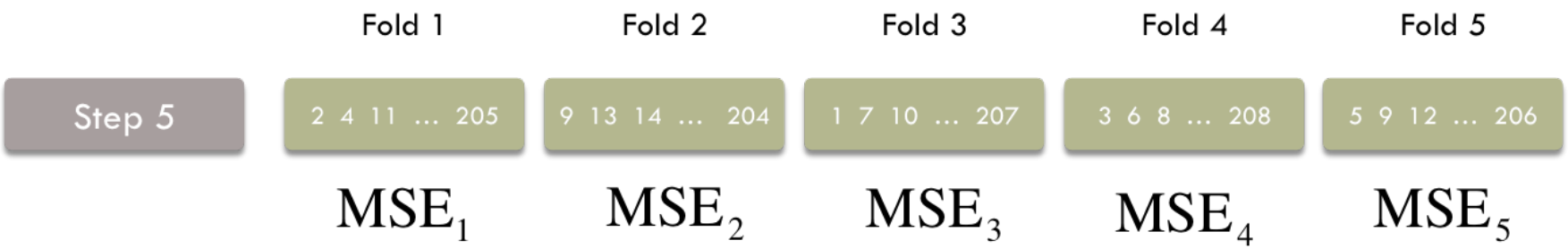
The Picture for 5-fold Cross-validation

1. Use Folds 1, 2, 3, 4 as a Train set to construct $\hat{f}$

2. Use Fold 5 as Test set to calculate error:

$$\mathrm{MSE}_5 = \sum_{i \in \text{Fold } 5} (y_i - \hat{f}(x_i))^2$$

The Picture for 5-fold Cross-validation



Form 5-fold CV estimate of prediction error: $CV_{(5)} = \frac{1}{5}\sum_{k=1}^{5} MSE_k$

Cross-validation standard error

- The K-fold CV estimate of prediction error is

$$\mathrm{CV}_{(K)} = \frac{1}{K} \sum_{k=1}^{K} \mathrm{MSE}_k$$

  where MSE_k is the error calculated on Fold k.
- It is also useful to calculate the standard error of the CV estimate
- The typical way of doing this: Calculate the sample standard deviation of $\{\mathrm{MSE}_1 \ldots, \mathrm{MSE}_K\}$, then divide by $\sqrt{K}$:[6]

$$\mathrm{SE}(\mathrm{CV}_{(K)}) = \frac{1}{\sqrt{K}} \mathrm{SD}(\mathrm{MSE}_1 \ldots, \mathrm{MSE}_K)$$

[6] This calculation isn't quite right, but it's a widely accepted approach for calculating standard errors for CV error estimates.

Back to the Automobile data

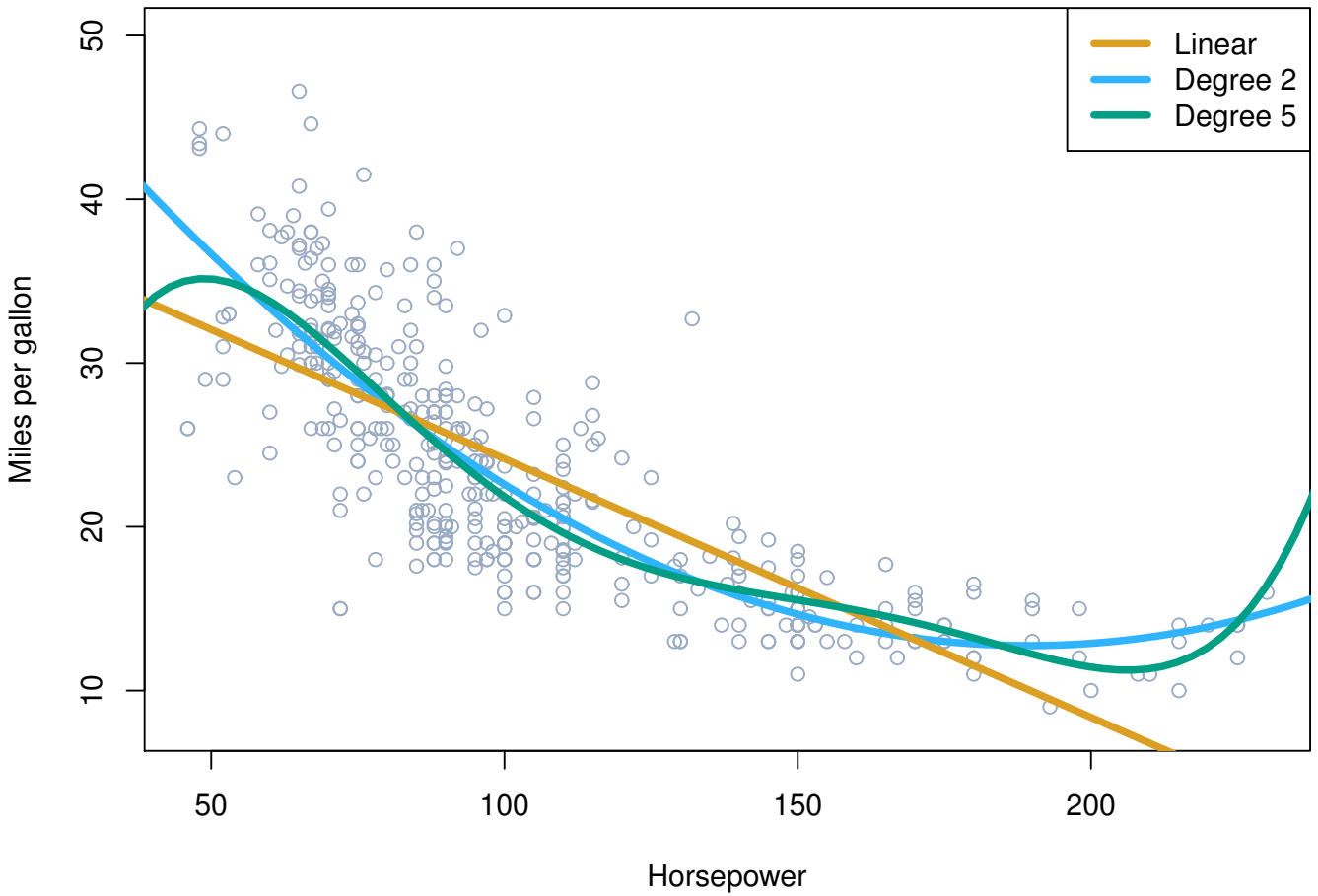


Figure: 3.8 from ISL. We want to figure out what degree polynomial we want to use to model the relationship between $Y =$ `Miles per gallon` and $X_1 =$ `Horsepower`

Example: Automobile data

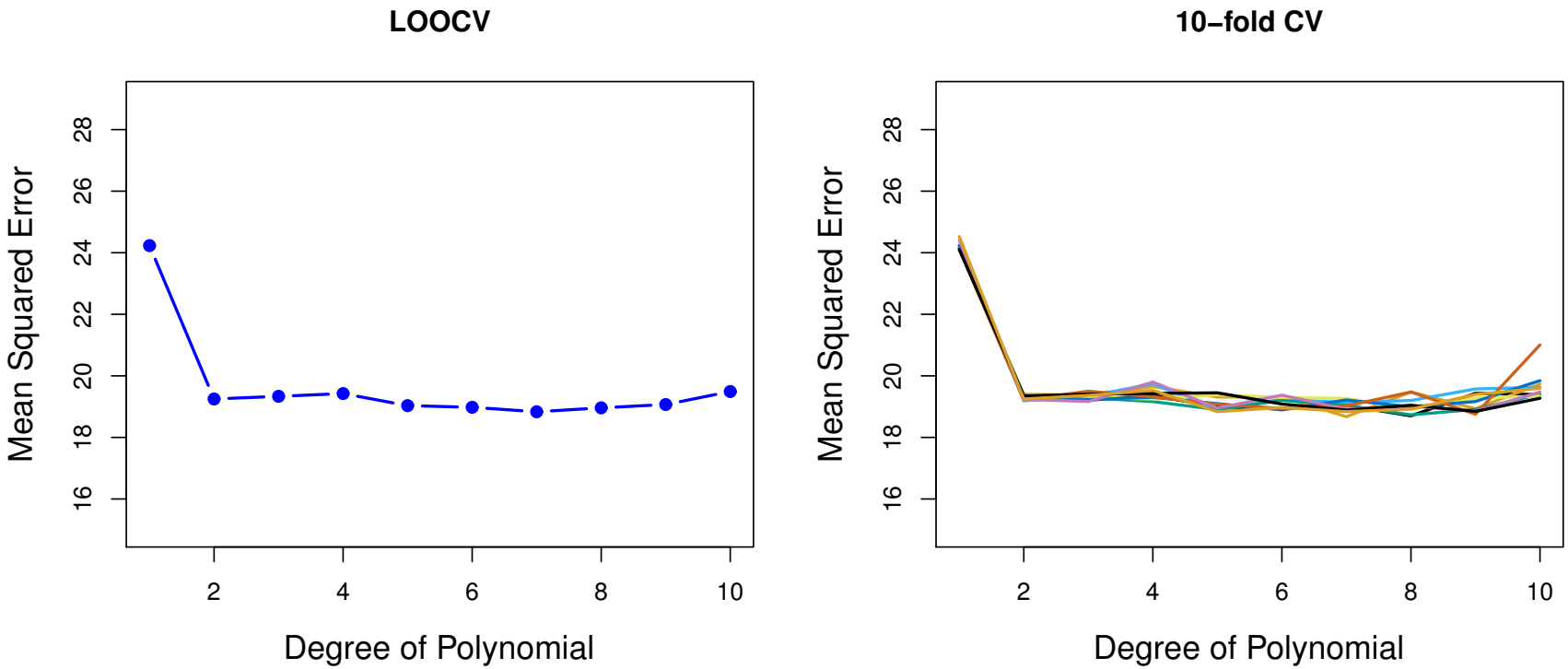
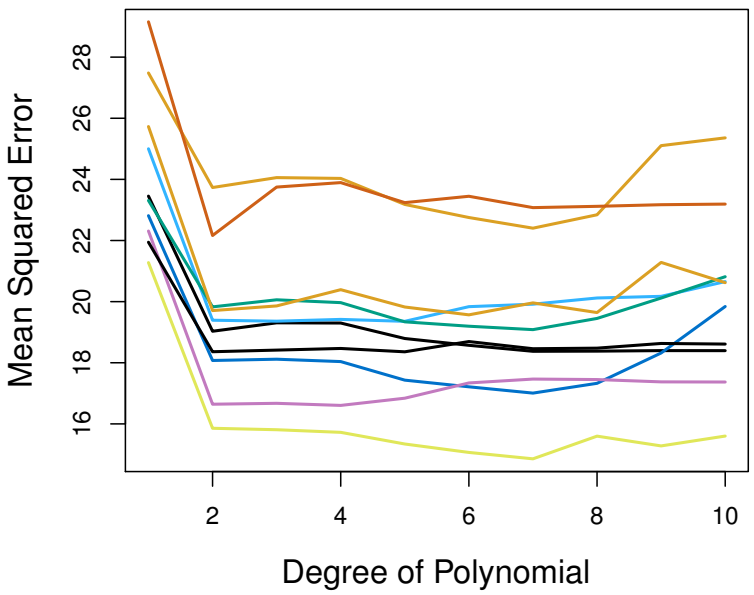
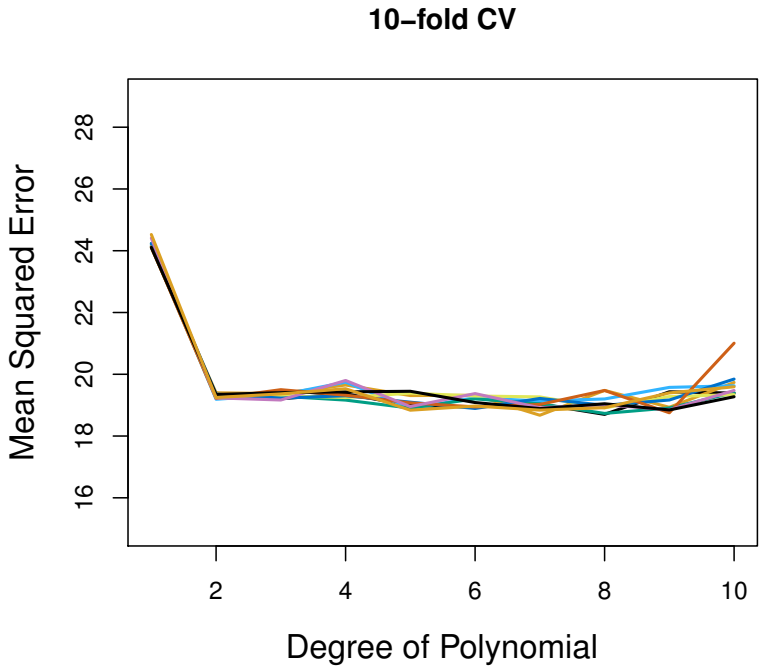


Figure 5.4 from ISL. Left panel shows estimated Test Error for LOOCV. Right panel shows estimated Test Error for 10*-fold CV run nine separate times.*

Same conclusion as Validation set approach: We should use a quadratic model

Validation set approach vs. 10-fold CV



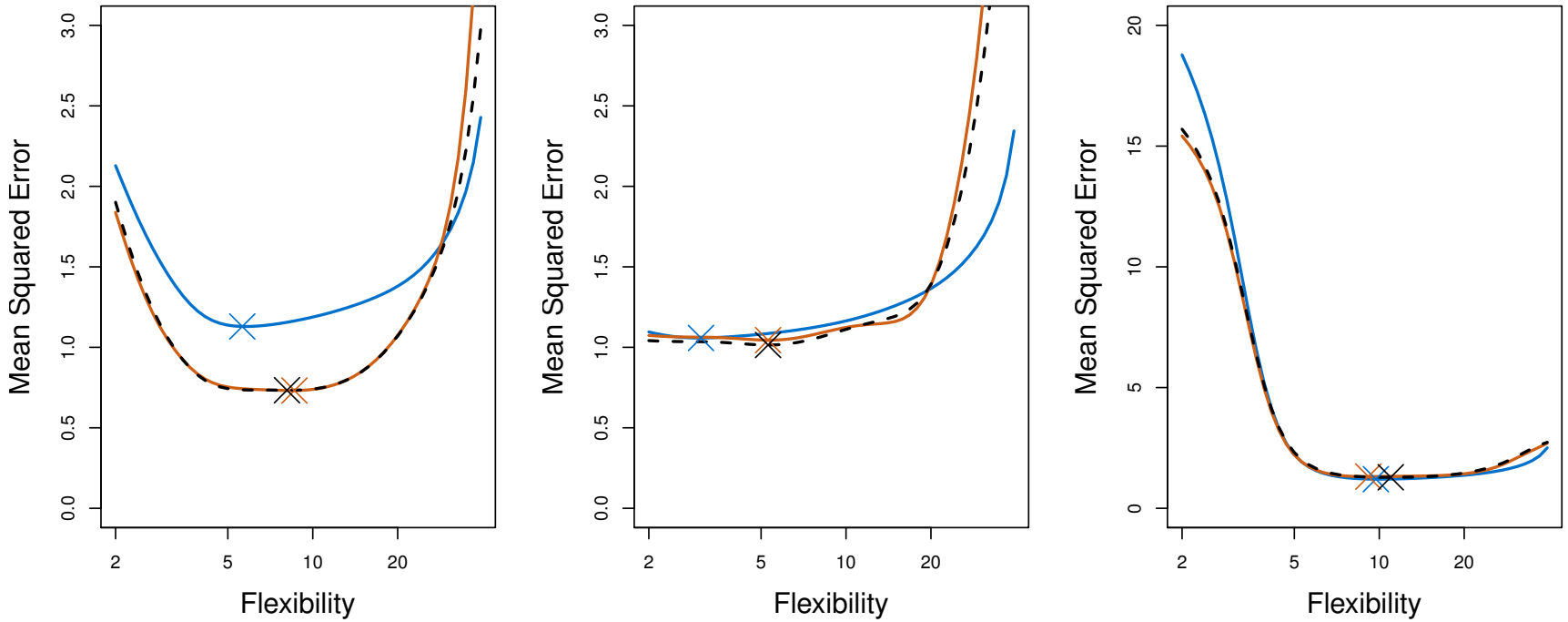


Validation set approach

10-fold CV

- Each plot shows estimated Test Error curves for multiple random splits of the data.
- The 10-fold CV error estimates are much more stable
- The Validation set error estimates are highly variable

CV error estimate vs. Actual test error



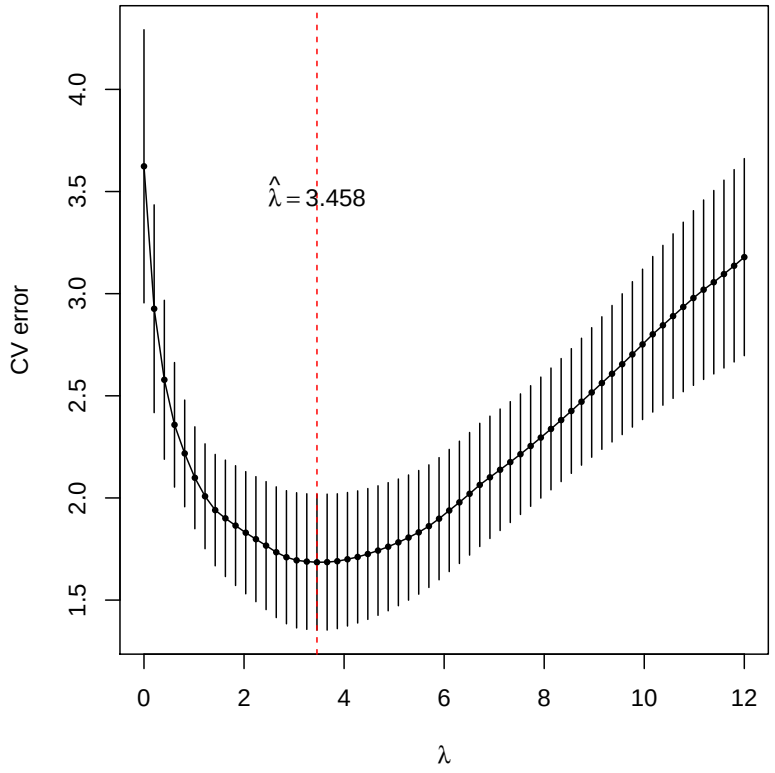
Blue curve: True Test Error

Dashed black curve: LOOCV estimate

Orange curve: 10-fold CV estimate

×'s: indicate *minimum* of each of the curves

The 1-standard error rule

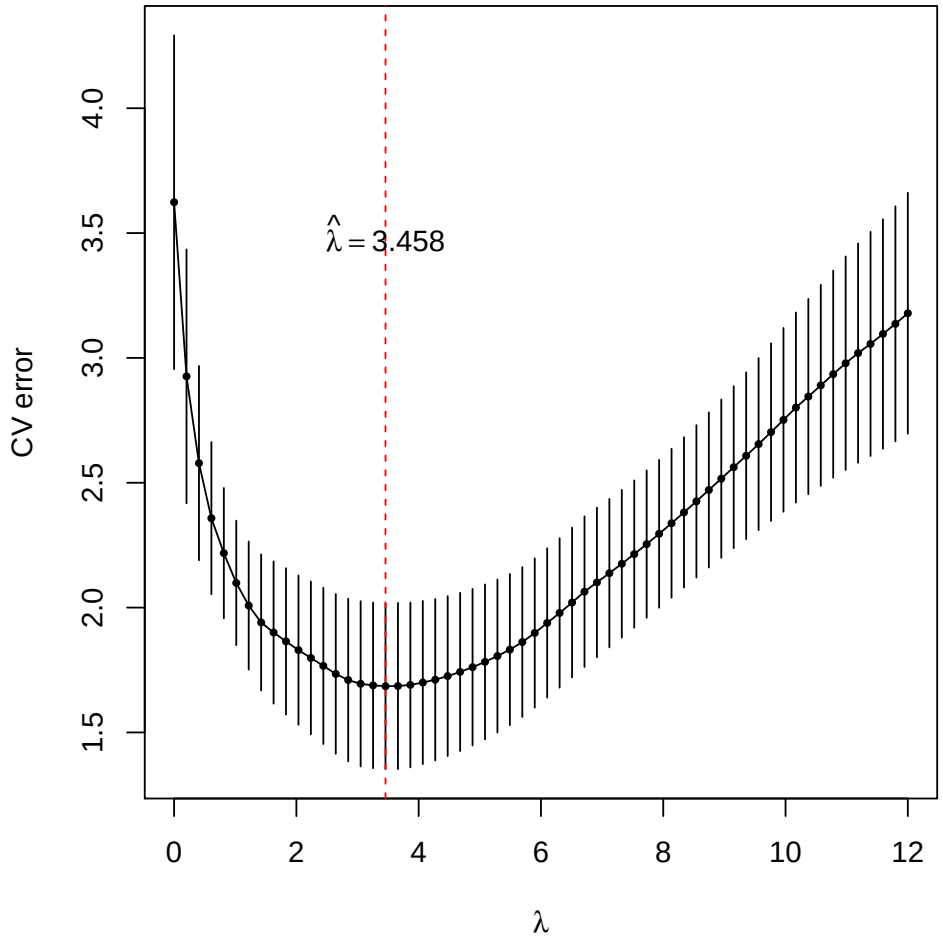


10-fold CV error curve as the tuning parameter λ varies

This plot shows CV error estimates and 1-standard-error bars for a bunch of different choices of a tuning parameter λ.[7]

[7] You can think of λ as the smoothing spline penalty. Large $\lambda \Rightarrow$ simpler model.

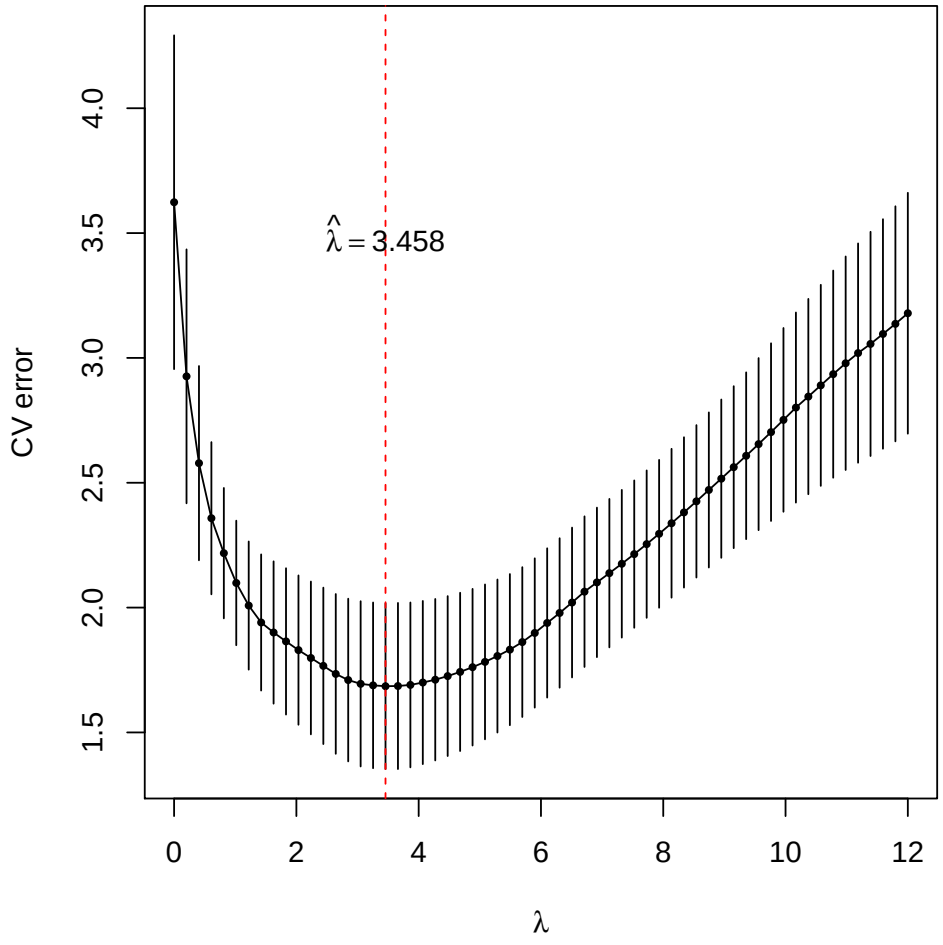
The 1-standard error rule



10-fold CV error curve as the tuning parameter λ varies

- $\lambda = 3.458$ gives us the model with the smallest estimated CV error.
- But we can see from the wide error bars that our prediction error estimates have high uncertainty.

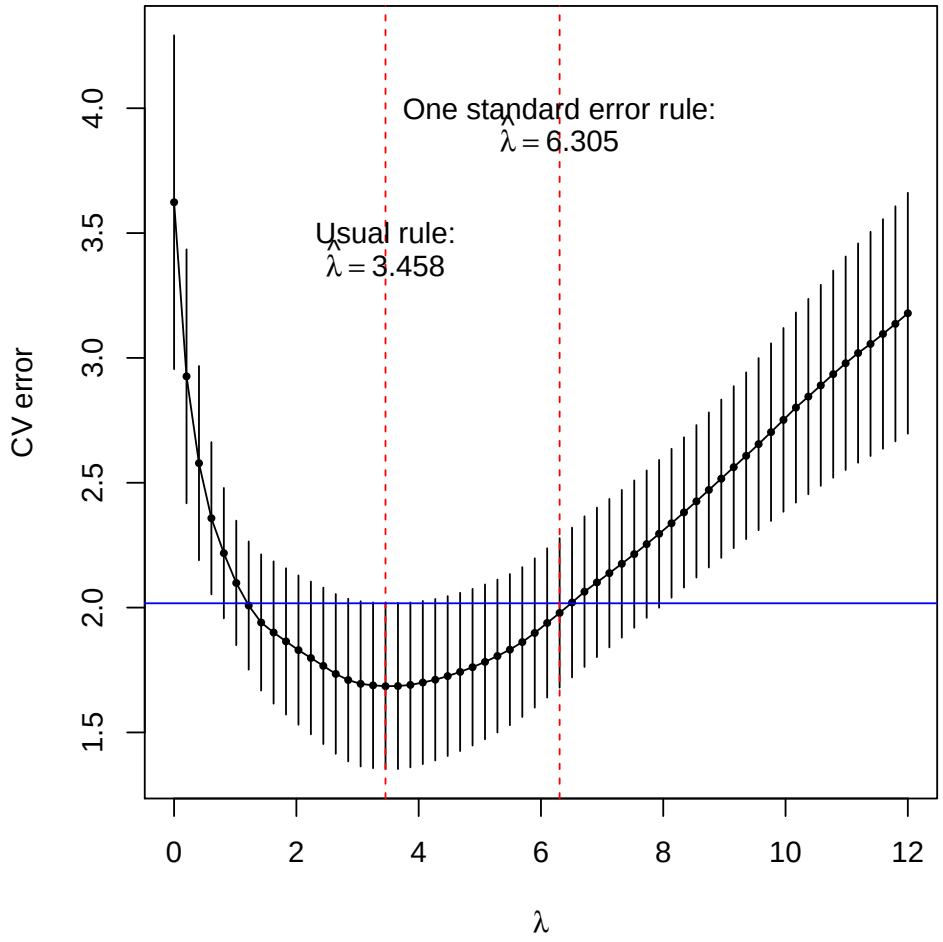
The 1-standard error rule



10-fold CV error curve as the tuning parameter λ varies

- The 1-standard error rule tells us to pick the *simplest model* whose CV error falls inside the 1-SE error bars of the lowest CV error model.

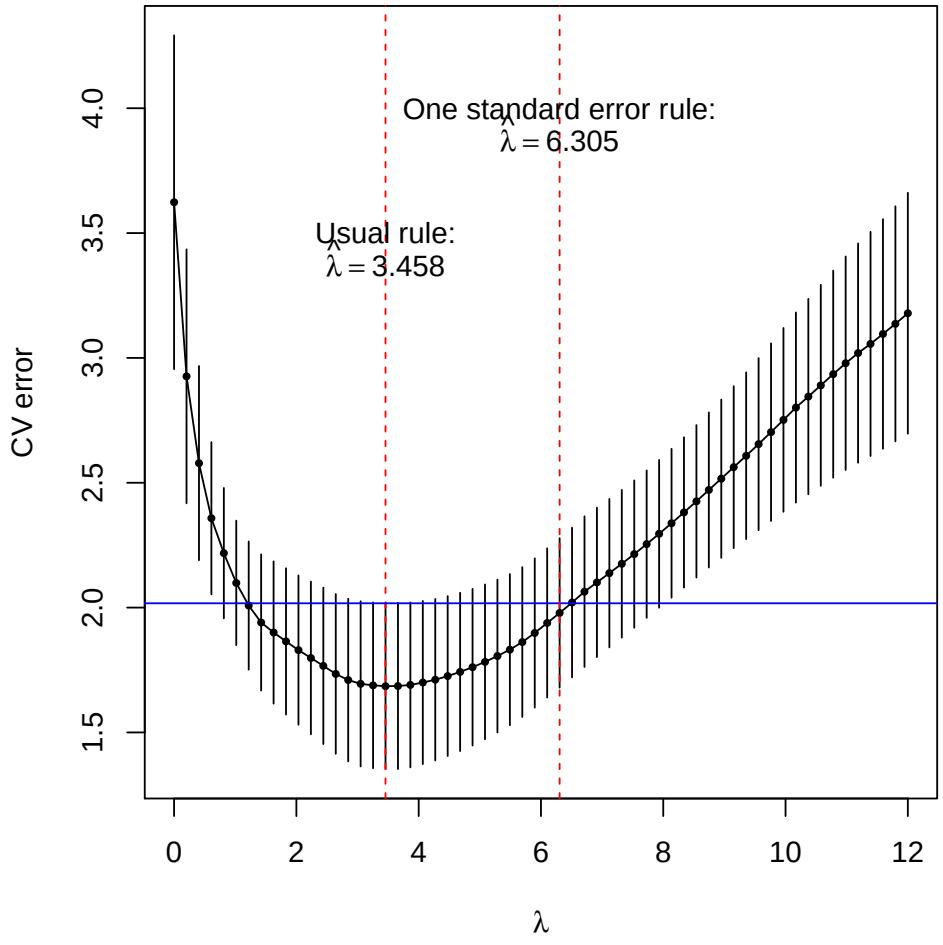
The 1-standard error rule



10-fold CV error curve as the tuning parameter λ varies

- The 1-standard error rule tells us to pick the *simplest model* whose CV error falls inside the 1-SE error bars of the lowest CV error model.

The 1-standard error rule

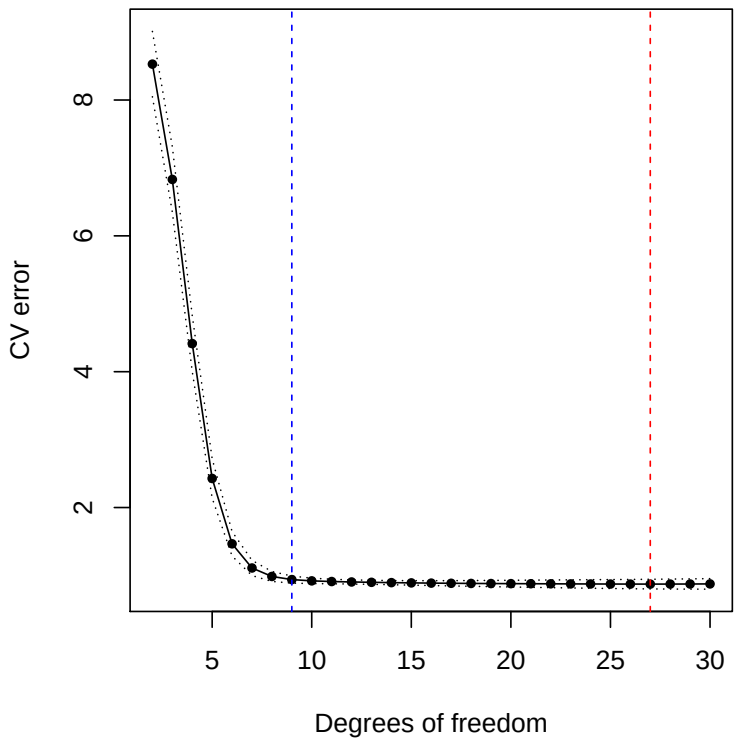


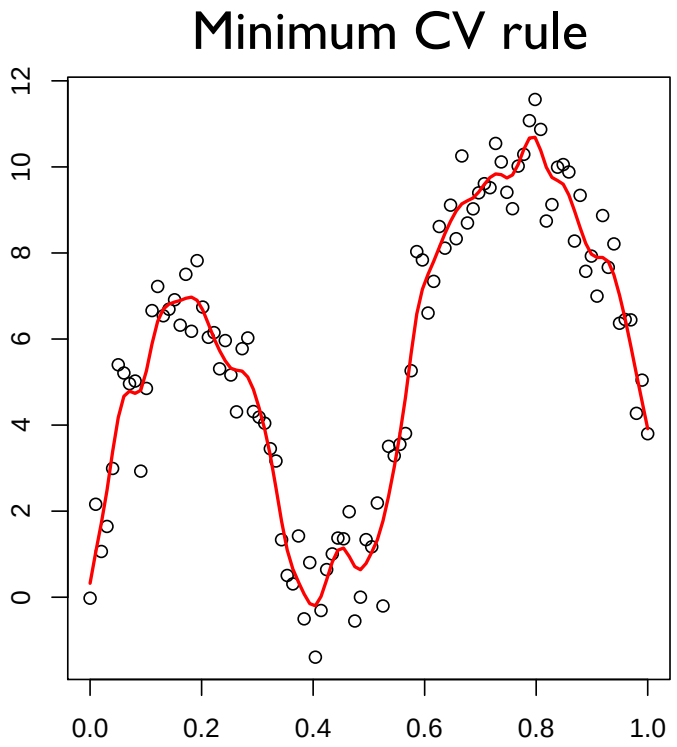
10-fold CV error curve as the tuning parameter λ varies

- Basic idea: We can't be certain that the $\lambda = 6.305$ model actually has higher prediction error than the $\lambda = 3.458$ model, so let's err on the side of caution and go with the *simpler* $\lambda = 6.305$ model.

Smoothing spline example

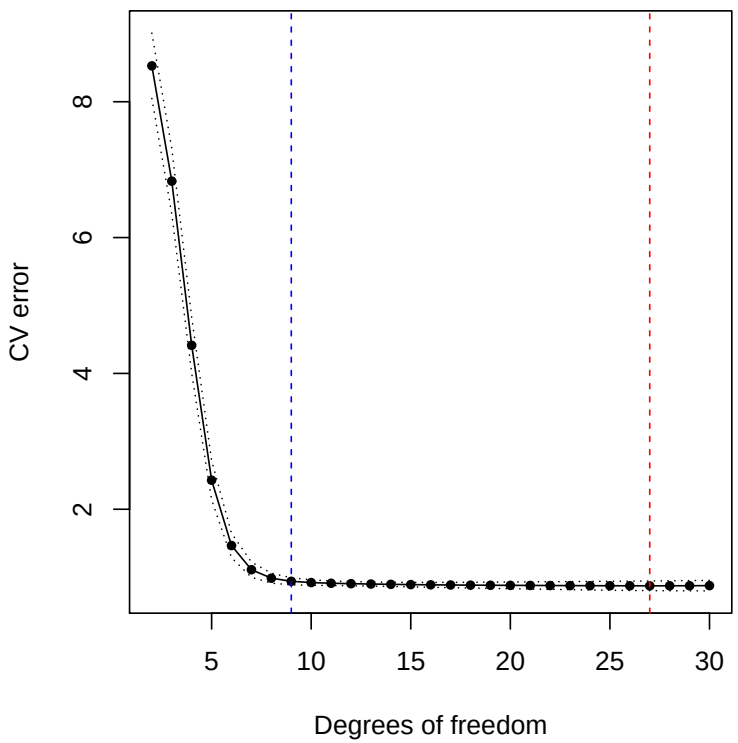
These plots show the results of applying 5-fold cross-validation to select the effective degrees of freedom for a smoothing spline fit to the points in the right panel.



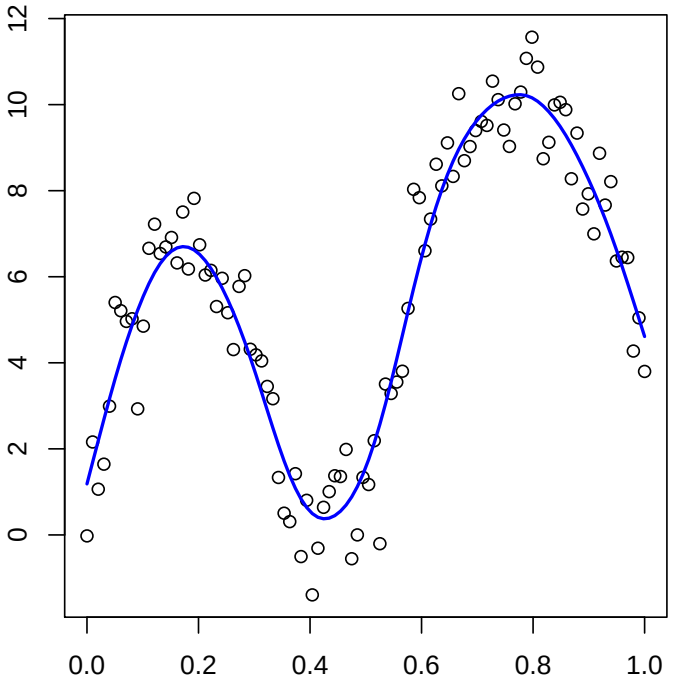


- Even at very large degrees of freedom, the smoothing spline is nicely behaved and has low CV error
- The minimum CV error rule selects a model with 27 degrees of freedom

Smoothing spline example



One standard error rule



- The one standard error rule selects a model with 9 degrees of freedom

Summary: Cross-validation

- We started with the question: *How do we pick the best model?*
- One answer: *Pick the model with the lowest prediction error.*
- The Validation set approach and K-fold Cross-validation are two resampling-based methods for estimating the *prediction error* of a model
- K-fold Cross-validation gives much more *stable* and *accurate* estimates of prediction error
- Once we get CV error estimates for the models we're considering, we can either:
  - Pick the model that has the minimum CV error; or
  - Use 1-SE rule and pick the *simplest* model whose error is within 1 standard error of the minimum CV error.
- From this we get: Our chosen model $\hat{f}$, *and* an estimate of its prediction error

Acknowledgements

All of the lectures notes for this class feature content borrowed with or without modification from the following sources:

- 36-462/36-662 Lecture notes (Prof. Tibshirani, Prof. G'Sell, Prof. Shalizi)
- 95-791 Lecture notes (Prof. Dubrawski)
- *An Introduction to Statistical Learning, with applications in R* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani
- *Applied Predictive Modeling*, (Springer, 2013), Max Kuhn and Kjell Johnson