

21) Regression Splines, Smoothing Splines, Local Regression

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Tables, Graphics, and Figures from
An Introduction to Statistical Learning

James et al. (2017): Chapters: 7.4, 7.5, 7.6, and
7.8.2

Piecewise Polynomials

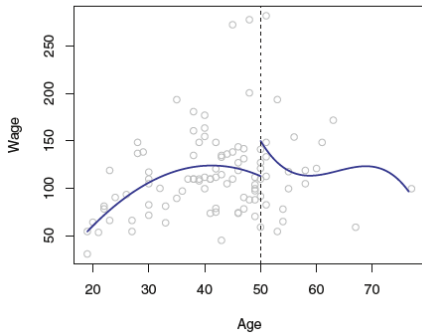
$$y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \beta_{31}x_i^3 + \epsilon_i & (I) \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \beta_{32}x_i^3 + \epsilon_i & (II) \end{cases}$$

(I) if $x_i < c$

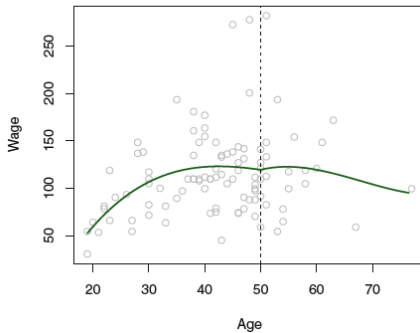
(II) if $x_i \geq c$

Unconstrained vs Constrained

Piecewise Cubic

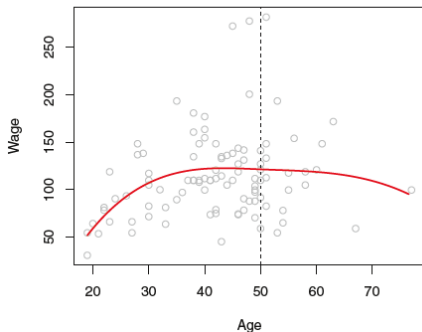


Continuous Piecewise Cubic

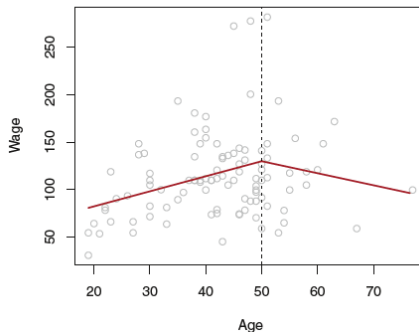


Continuous, Continuous First and Second Derivatives vs Linear Continuous

Cubic Spline



Linear Spline



Cubic Spline Basis Representation

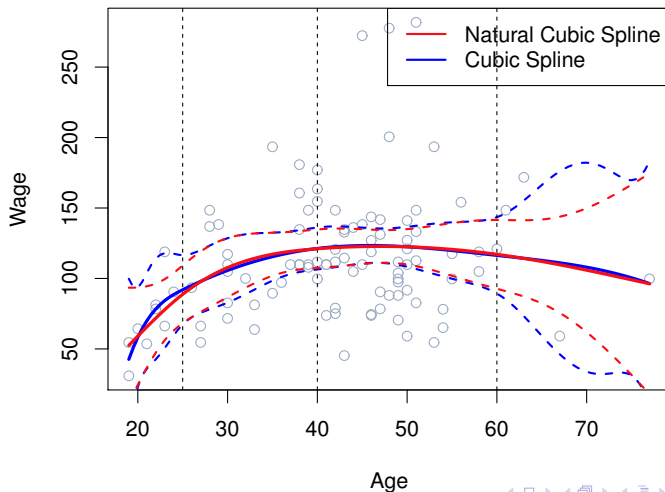
$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \dots + \beta_{k+3} b_{k+3}(x_i) + \epsilon_i$$

$$h(x, \xi) = (x - \xi)_+^3 = \begin{cases} (x - \xi)^3 & \text{if } x > \xi \\ 0 & \text{otherwise} \end{cases}$$

Intercept and 3+K Predictors:

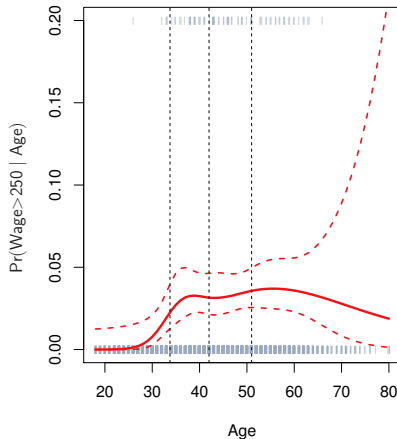
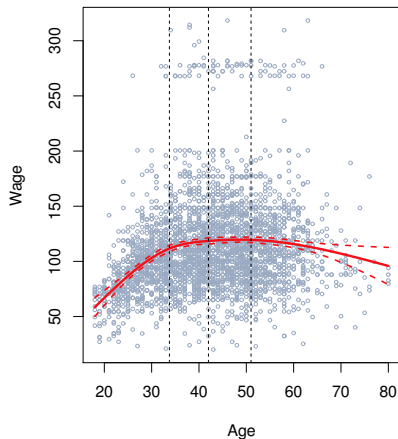
$$1, X, X^2, X^3, h(x, \xi_1), h(x, \xi_2), \dots, h(x, \xi_K)$$

Three Knots

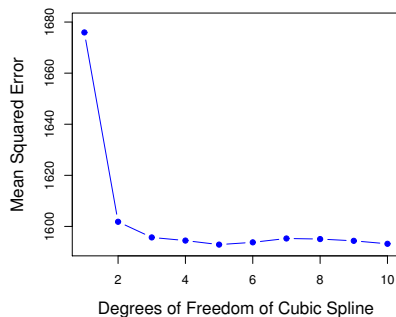
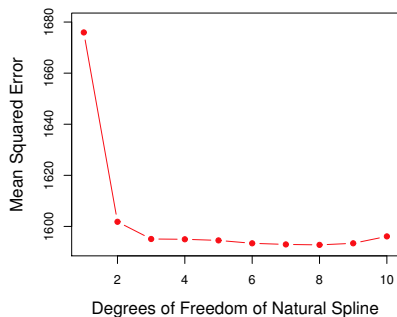


Spline with Three Knots (25th, 50th, and 75th) vs Logistic Regression

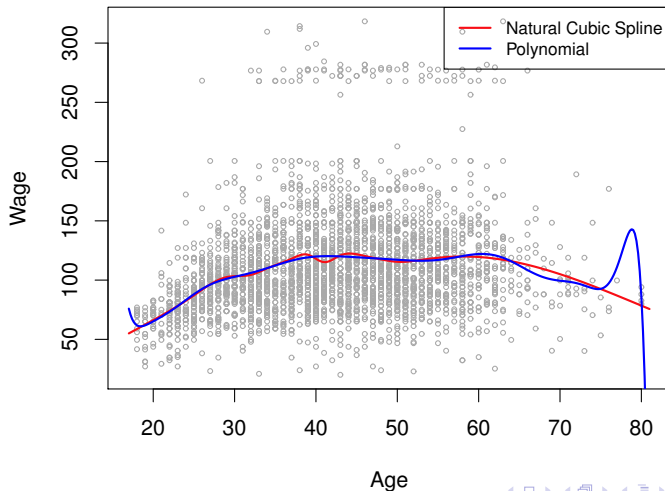
Natural Cubic Spline



Ten-fold Cross-Validation



Spline with 15 df vs Degree-15 Polynomial



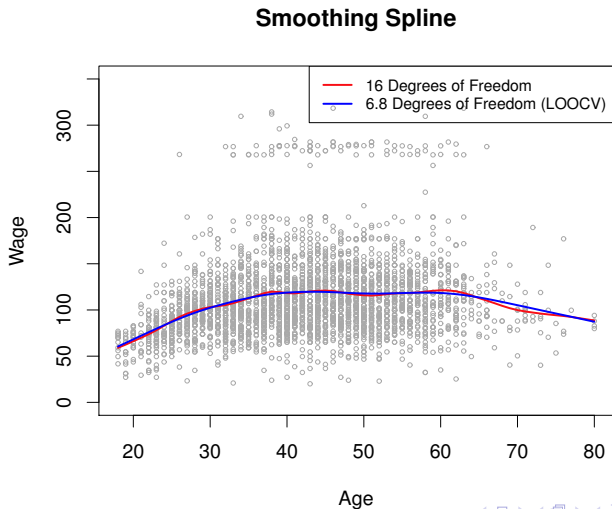
Smoothing Splines

$$\sum_{i=1}^n (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

$$\hat{g}_\lambda = S_\lambda y, \quad df_\lambda = \sum_{i=1}^n \{S_\lambda\}_{ii}$$

$$\begin{aligned} RSS_{cv}(\lambda) &= \sum_{i=1}^n (y_i - \hat{g}_\lambda^{(-i)}(x_i))^2 \\ &= \sum_{i=1}^n \left[\frac{y_i - \hat{g}_\lambda(x_i)}{1 - \{S_\lambda\}_{ii}} \right]^2 \end{aligned}$$

16 Effective df vs 6.8 Effective df Resulted by Leave-One-Out Cross-Validation



library(ISLR); attach(Wage)

```
agelims=range(age)
```

```
age.grid=seq(from=agelims[1],to=agelims[2])
```

```
library(splines)
```

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

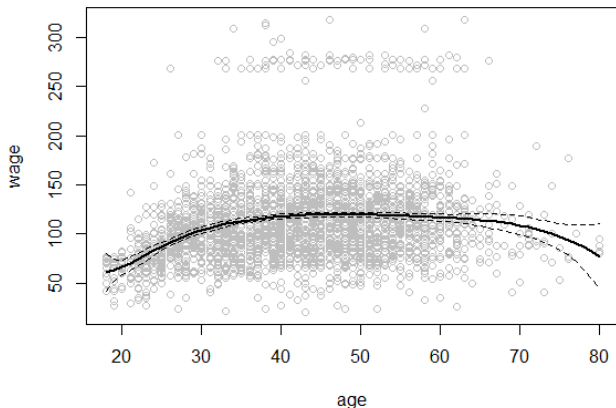
```
pred=predict(fit,newdata=list(age=age.grid),se=T)
```

```
plot(age,wage,col="gray");
```

```
lines(age.grid,pred$fit,lwd=2)
```

```
lines(age.grid,pred$fit+2*pred$se,lty="dashed")
```

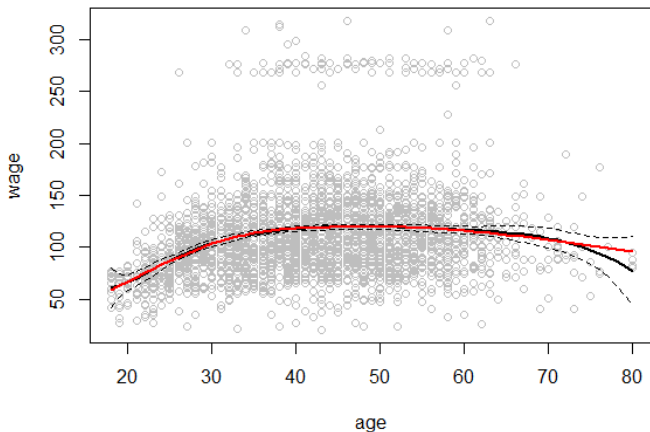
```
lines(age.grid,pred$fit-2*pred$se,lty="dashed")
```



```
fit2=lm(wage~ns(age,df=4),data=Wage)
```

```
pred2=predict(fit2,newdata=list(age=age.grid),se=T)
```

```
lines(age.grid, pred2$fit,col="red",lwd=2)
```



```
plot(age,wage,xlim=agelims,cex=.5,col="darkgrey")
```

```
title("Smoothing Spline")
```

```
fit=smooth.spline(age,wage,df=16)
```

```
fit2=smooth.spline(age,wage,cv=TRUE)
```

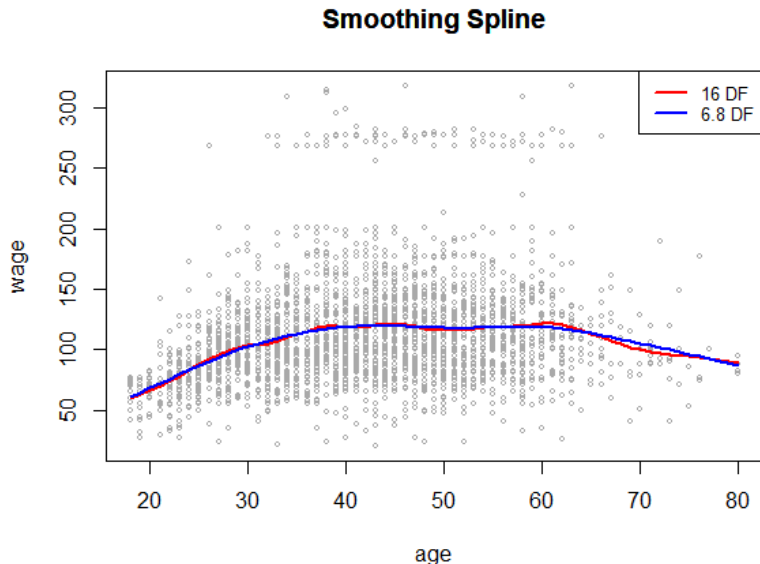
```
fit2$df
```

```
lines(fit,col="red",lwd=2)
```

```
lines(fit2,col="blue",lwd=2)
```

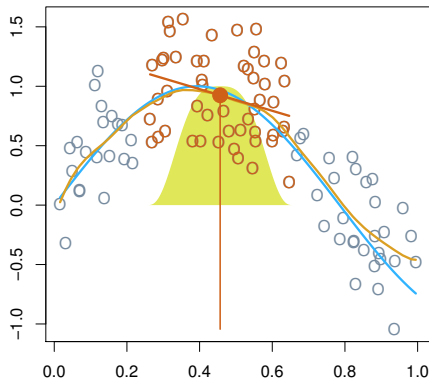
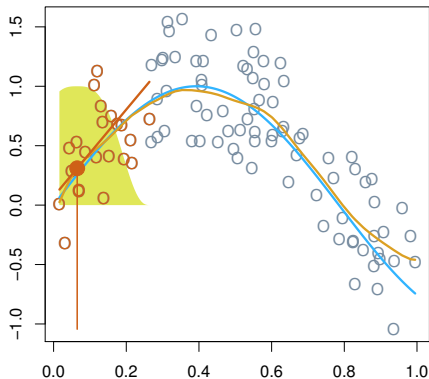
```
legend("topright",legend=c("16 DF", "6.8 DF"),  
col=c("red","blue"), lty=1,lwd=2,cex=.8)
```


df =16 vs Cross-Validation



Local Regression - Simulated Data

Local Regression



Local Regression at $X = x_0$

1. Gather $s = \frac{k}{n}$ training points whose x_i are closer to x_0
2. Assign a weight $K_{i0} = K(x_i, x_0)$
3. Fit $\sum_{i=1}^n K_{i0}(y_i - \beta_0 - \beta_1 x_i)^2$
4. Fitted value at x_0 is $\hat{f}(x_0) = \hat{\beta}_0 - \hat{\beta}_1 x_0$

```
plot(age,wage,xlim=agelims,cex=.5,col="darkgrey")
```

```
title("Local Regression")
```

```
fit=loess(wage~age,span=.2,data=Wage)
```

```
fit2=loess(wage~age,span=.5,data=Wage)
```

```
lines(age.grid,predict(fit,data.frame(age=age.grid)),  
col="red",lwd=2)
```

```
lines(age.grid,predict(fit2,data.frame(age=age.grid)),  
col="blue",lwd=2)
```

```
legend("topright",legend=c("Span=0.2","Span=0.5"),  
col=c("red","blue"),lty=1,lwd=2,cex=.8)
```

Neighborhood of 20% vs 50% of the Observations

Local Regression

