16) Regression Splines

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Reference

Tables, Graphics, and Figures from

An Introduction to Statistical Learning

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

Hastie et al. (2017): Ch 5

Basis Functions

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + ... + \beta_k b_k(x_i) + \epsilon_i$$

$$b_j(x_i) = x_i^j$$

$$b_j(x_i) = I(c_j \leq x_i < c_{j+1})$$

Piecewise Cubic Polynomial

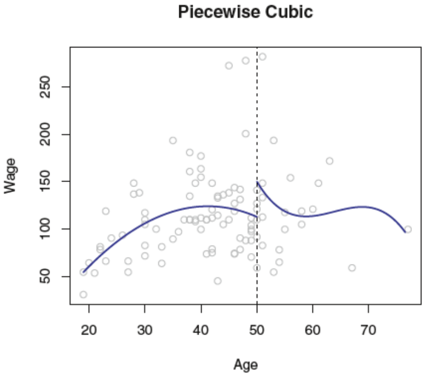
$$y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \beta_{31}x_i^3 + \epsilon_i & (I) \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \beta_{32}x_i^3 + \epsilon_i & (II) \end{cases}$$

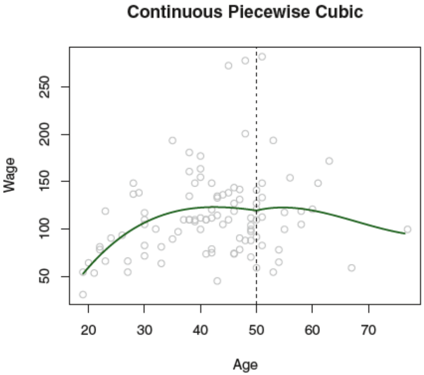
$$(I) \ if \ x_i < c$$

$$(II) \ if \ x_i \geq c$$

8 df = 4 parameters each side

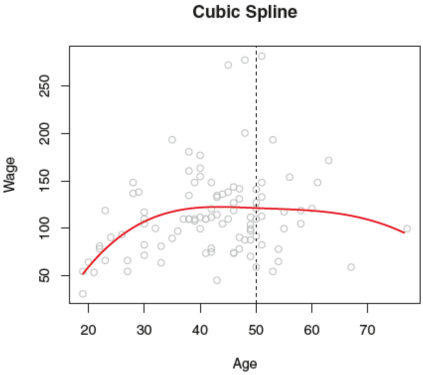
Unconstrained (8 df) vs Constrained (7 df)

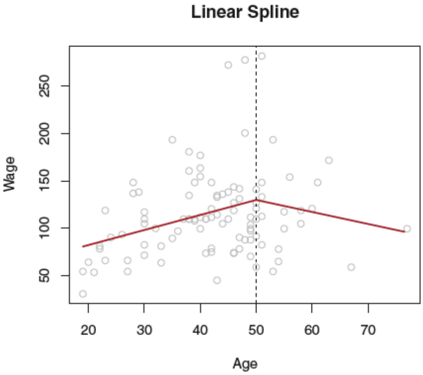




Continuous, Continuous First and Second Derivatives vs Linear Continuous

(5 df = 8 - 3) vs (3 df = 4 - 1)





Truncated Power Basis Function per Knot

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

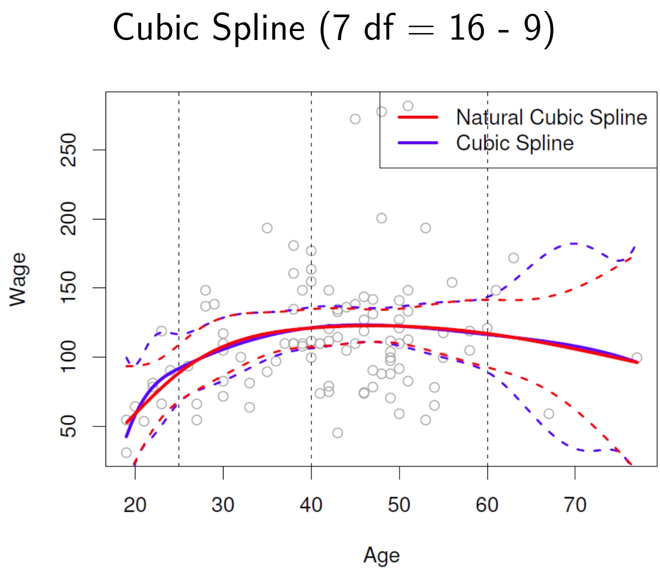
$$h(x, \xi) = (x - \xi)^3_+ = \begin{cases} (x - \xi)^3 & \textit{if} \quad x > \xi \\ 0 & \textit{otherwise} \end{cases}$$

Discontinuity in only the Third Derivative

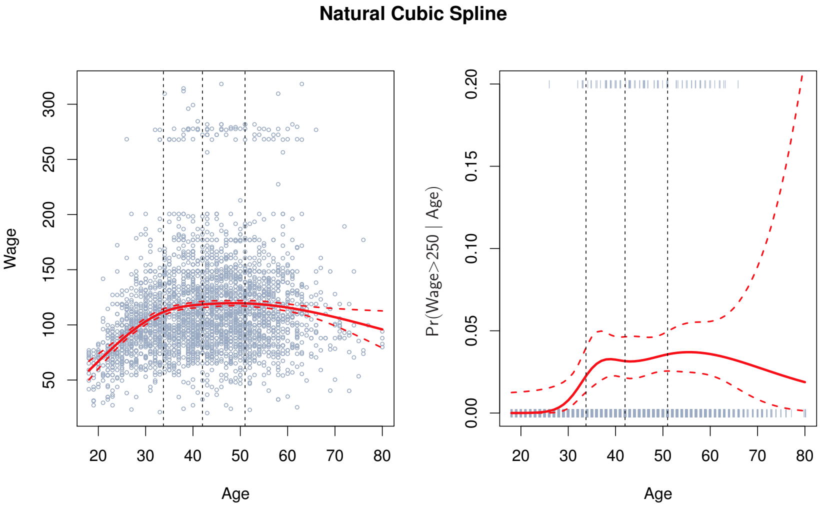
Cubic Spline with K knots: K+4 df

$$\underset{\textit{regions}}{2} \times \underset{\textit{parameters}}{4} - \underset{\textit{knots}}{1} \times \underset{\textit{constraints}}{3} = 5 \text{ df}$$

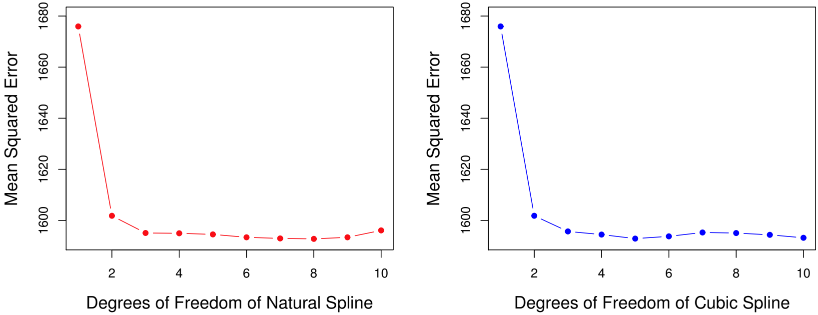
Natural Cubic Spline (5 df = 16 - 9 - 2)



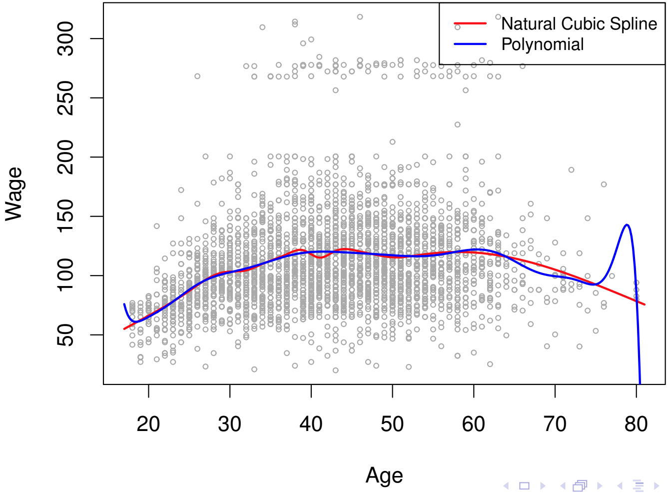
Spline with Three Knots (25th, 50th, and 75th) vs Logistic Regression



Ten-fold Cross-Validation



Spline with 15 df vs Degree-15 Polynomial



Smoothing Splines

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

$$f(x) = \sum_{j=1}^{N} N_j(x)\theta_j$$

$$(y - N\theta)^T (y - N\theta) + \lambda \theta^T \Omega_N \theta$$

$$\hat{\theta} = (N^T N + \lambda \Omega_N)^{-1} N^T y$$

Leave-one-out Cross-Validation

$$\hat{f} = N(N^T N + \lambda \Omega_N)^{-1} N^T y$$

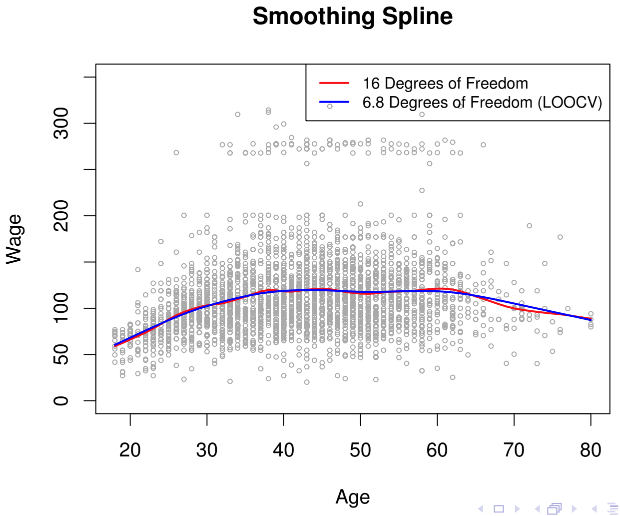
$$\hat{f} = S_\lambda y$$

$$df_\lambda = trace(S_\lambda)$$

$$CV(\hat{f}_\lambda) = \frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{f}_\lambda^{(-i)}(x_i))^2$$

$$= \frac{1}{N} \sum_{i=1}^{N} [\frac{y_i - \hat{f}_\lambda(x_i)}{1 - S_\lambda(i,i)}]^2$$

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])
```

 # Default: Cubic Spline with no Intercept

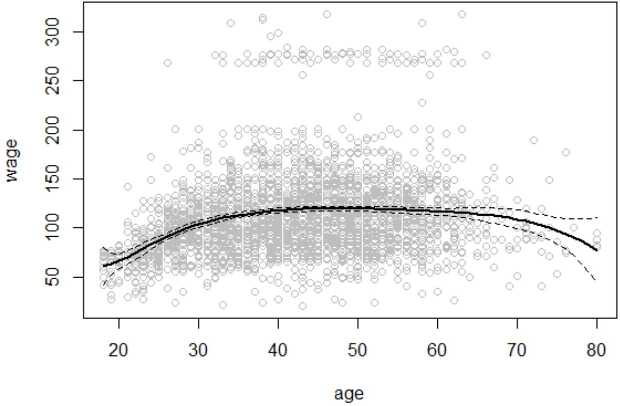
```
library(splines)
fit=lm(wage~bs(age,knots=c(25,40,60)),data=Wage)
pred=predict(fit,newdata=list(age=age.grid),se=T)
```

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")



For “bs”: df = degree of freedom - 1

```
dim(bs(age,knots=c(25,40,60)))
```

3000 6

```
attr(bs(age,df=6),"knots")
```

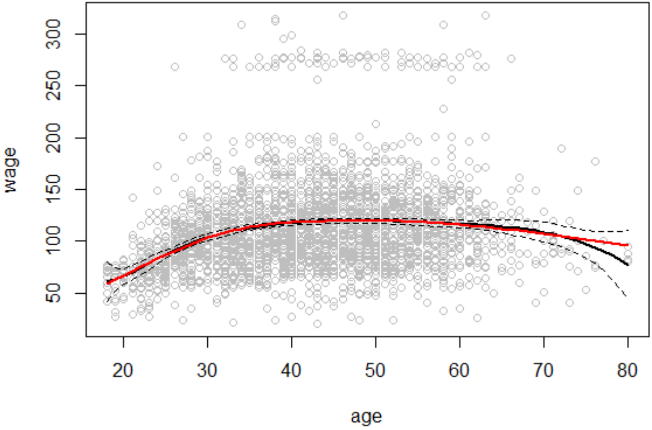
25%	50%	75%
33.75	42.00	51.00

```
attr(bs(age,df=7),"knots")
```

20%	40%	60%	80%
32	39	46	53

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