21) Regression Splines

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March 2018

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

Hastie et al. (2017): Chapter: 5

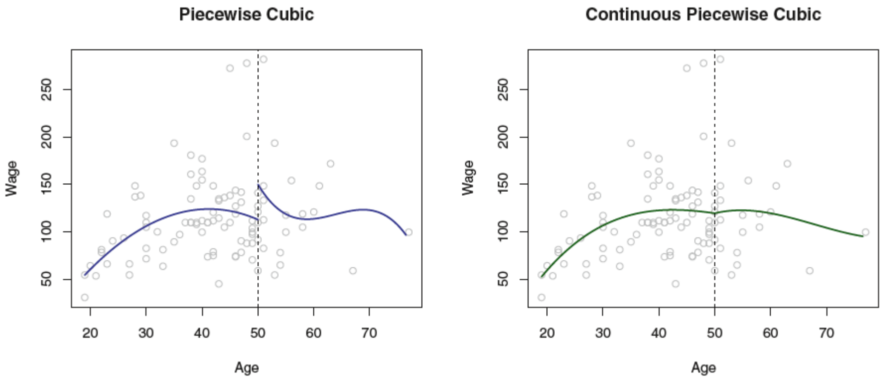
Piecewise Polynomials

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

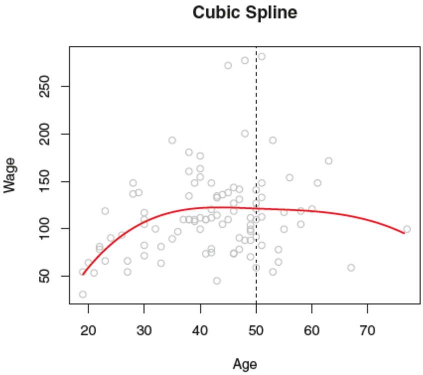
$$(I) \text{ } if \text{ } x_i < c$$

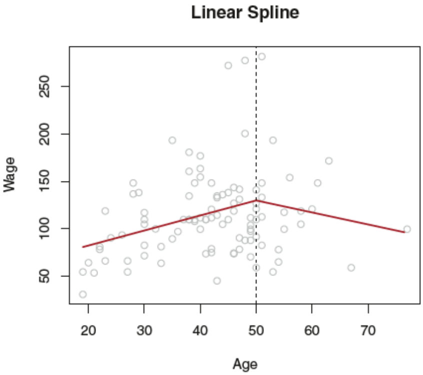
$$(II) \text{ } if \text{ } x_i \geq c$$

Unconstrained vs Constrained



Continuous, Continuous First and Second Derivatives vs Linear Continuous





Cubic Spline Basis Representation

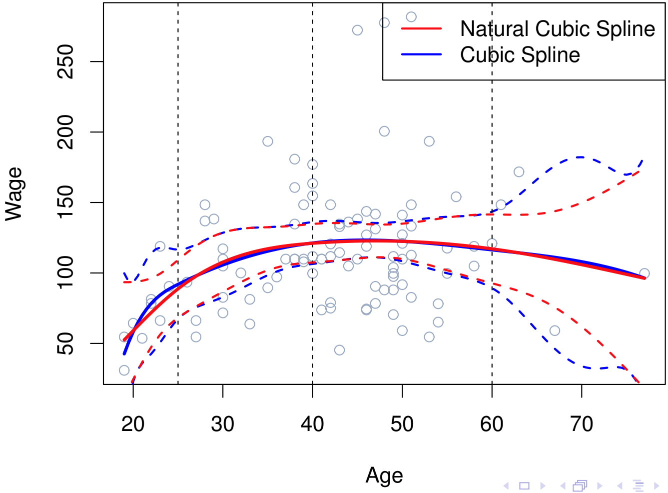
$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \ldots + \beta_{k+3} b_{k+3}(x_i) + \epsilon_i$$

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

Intercept and 3+K Predictors:

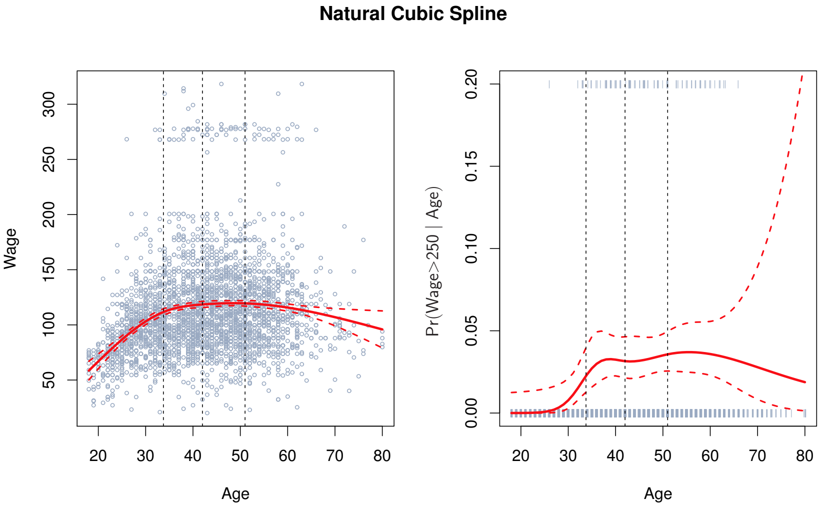
$$1, X, X^2, X^3, h(x, \xi_1), h(x, \xi_2), \ldots, h(x, \xi_K)$$

Three Knots

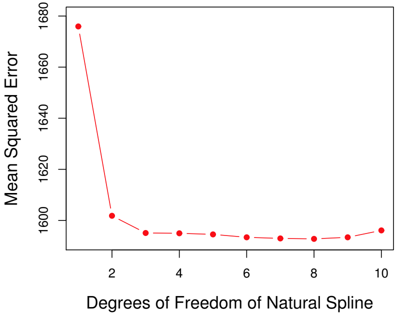


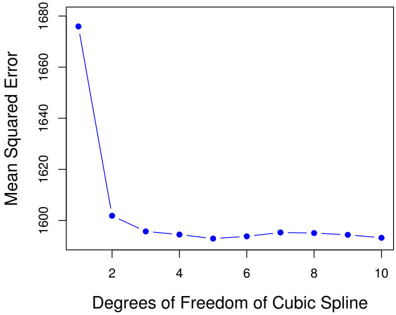
Natural Cubic Spline
Cubic Spline
Wage
Age
50
100
150
200
250
20
30
40
50
60
70

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

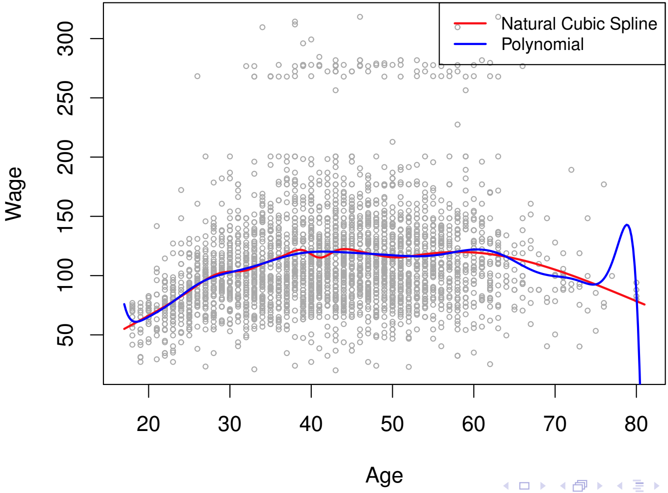


Ten-fold Cross-Validation





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

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

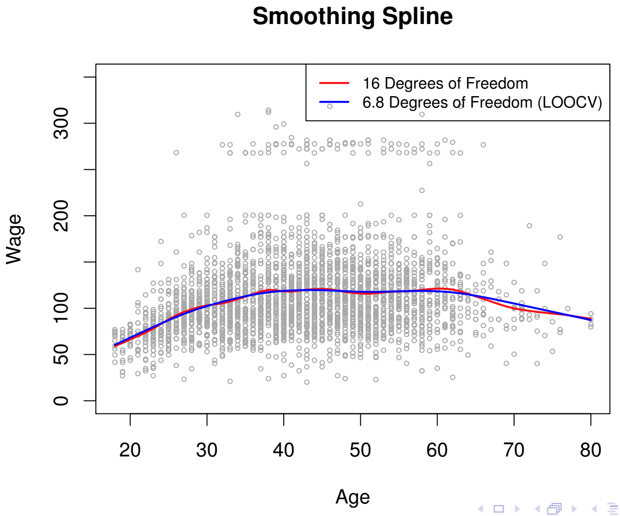
$$\hat{f} = S_\lambda y$$

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

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

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

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



library(ISLR); attach(Wage)

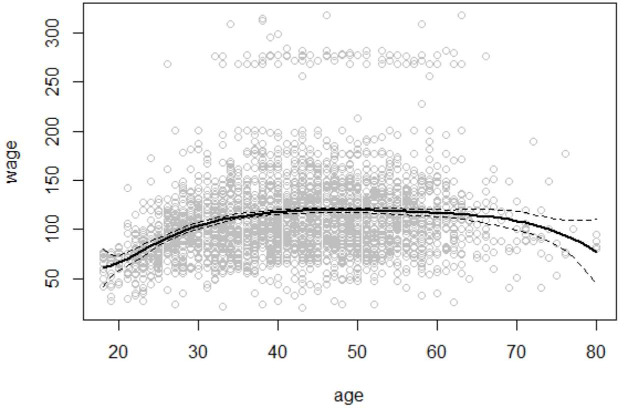
```
agelims=range(age)
age.grid=seq(from=agelims[1],to=agelims[2])

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")

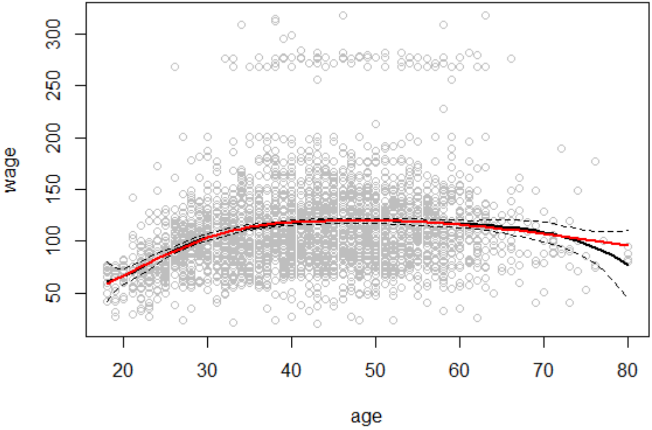
lines(age.grid,pred$fit-2*pred$se,lty="dashed")



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