

Cubic Splines

A cubic spline with knots at ξ_k , $k = 1, \dots, K$ is a piecewise cubic polynomial with continuous derivatives up to order 2 at each knot.

Again we can represent this model with truncated power basis functions

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_{K+3} b_{K+3}(x_i) + \epsilon_i,$$

$$b_1(x_i) = x_i$$

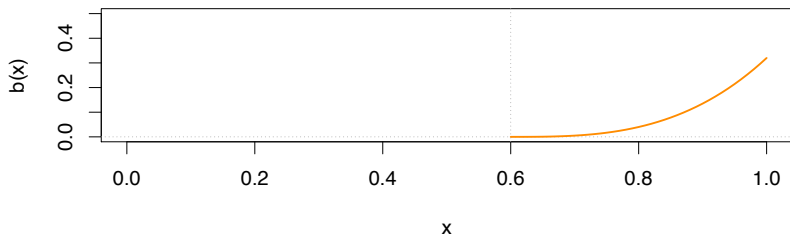
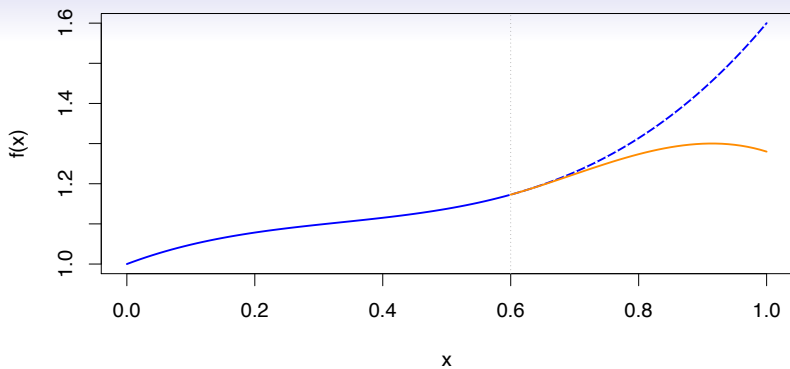
$$b_2(x_i) = x_i^2$$

$$b_3(x_i) = x_i^3$$

$$b_{k+3}(x_i) = (x_i - \xi_k)_+^3, \quad k = 1, \dots, K$$

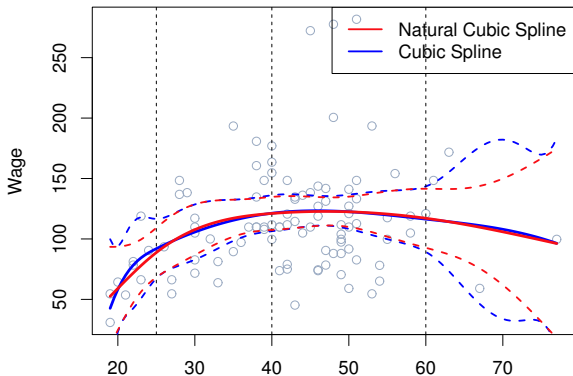
where

$$(x_i - \xi_k)_+^3 = \begin{cases} (x_i - \xi_k)^3 & \text{if } x_i > \xi_k \\ 0 & \text{otherwise} \end{cases}$$



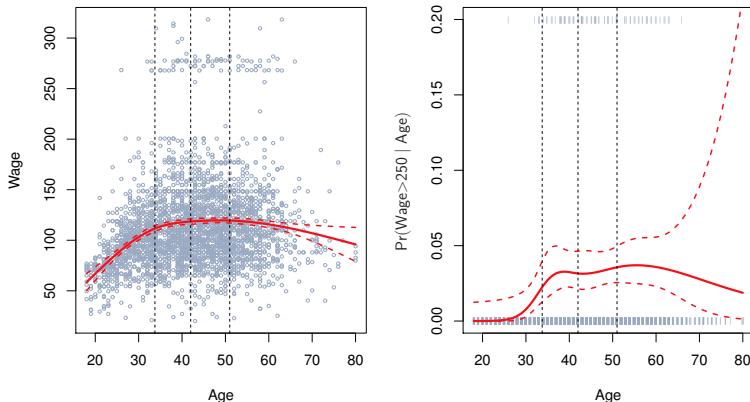
Natural Cubic Splines

A natural cubic spline extrapolates linearly beyond the boundary knots. This adds $4 = 2 \times 2$ extra constraints, and allows us to put more internal knots for the same degrees of freedom as a regular cubic spline.



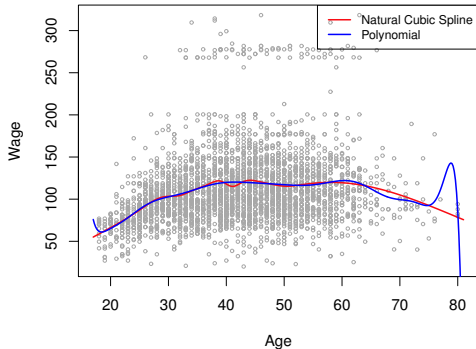
Fitting splines in R is easy: `bs(x, ...)` for any degree splines, and `ns(x, ...)` for natural cubic splines, in package `splines`.

Natural Cubic Spline



Knot placement

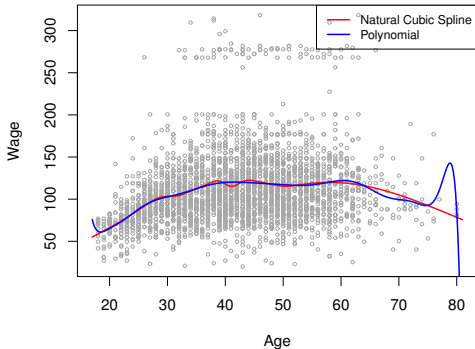
- One strategy is to decide K , the number of knots, and then place them at appropriate quantiles of the observed X .
- A cubic spline with K knots has $K + 4$ parameters or degrees of freedom.
- A natural spline with K knots has K degrees of freedom.



Comparison of a degree-14 polynomial and a natural cubic spline, each with 15df.

Knot placement

- One strategy is to decide K , the number of knots, and then place them at appropriate quantiles of the observed X .
- A cubic spline with K knots has $K + 4$ parameters or degrees of freedom.
- A natural spline with K knots has K degrees of freedom.



Comparison of a degree-14 polynomial and a natural cubic spline, each with 15df.

```
ns(age, df=14)  
poly(age, deg=14)
```

Smoothing Splines

This section is a little bit mathematical



Consider this criterion for fitting a smooth function $g(x)$ to some data:

$$\underset{g \in \mathcal{S}}{\text{minimize}} \sum_{i=1}^n (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

Smoothing Splines

This section is a little bit mathematical



Consider this criterion for fitting a smooth function $g(x)$ to some data:

$$\underset{g \in \mathcal{S}}{\text{minimize}} \sum_{i=1}^n (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

- The first term is RSS, and tries to make $g(x)$ match the data at each x_i .

Smoothing Splines

This section is a little bit mathematical



Consider this criterion for fitting a smooth function $g(x)$ to some data:

$$\underset{g \in \mathcal{S}}{\text{minimize}} \sum_{i=1}^n (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

- The first term is RSS, and tries to make $g(x)$ match the data at each x_i .
- The second term is a *roughness penalty* and controls how wiggly $g(x)$ is. It is modulated by the *tuning parameter* $\lambda \geq 0$.

Smoothing Splines

This section is a little bit mathematical



Consider this criterion for fitting a smooth function $g(x)$ to some data:

$$\underset{g \in \mathcal{S}}{\text{minimize}} \sum_{i=1}^n (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

- The first term is RSS, and tries to make $g(x)$ match the data at each x_i .
- The second term is a *roughness penalty* and controls how wiggly $g(x)$ is. It is modulated by the *tuning parameter* $\lambda \geq 0$.
 - The smaller λ , the more wiggly the function, eventually interpolating y_i when $\lambda = 0$.

Smoothing Splines

This section is a little bit mathematical



Consider this criterion for fitting a smooth function $g(x)$ to some data:

$$\underset{g \in \mathcal{S}}{\text{minimize}} \sum_{i=1}^n (y_i - g(x_i))^2 + \lambda \int g''(t)^2 dt$$

- The first term is RSS, and tries to make $g(x)$ match the data at each x_i .
- The second term is a *roughness penalty* and controls how wiggly $g(x)$ is. It is modulated by the *tuning parameter* $\lambda \geq 0$.
 - The smaller λ , the more wiggly the function, eventually interpolating y_i when $\lambda = 0$.
 - As $\lambda \rightarrow \infty$, the function $g(x)$ becomes linear.

Smoothing Splines continued

The solution is a natural cubic spline, with a knot at every unique value of x_i . The roughness penalty still controls the roughness via λ .

Smoothing Splines continued

The solution is a natural cubic spline, with a knot at every unique value of x_i . The roughness penalty still controls the roughness via λ .

Some details

- Smoothing splines avoid the knot-selection issue, leaving a single λ to be chosen.

Smoothing Splines continued

The solution is a natural cubic spline, with a knot at every unique value of x_i . The roughness penalty still controls the roughness via λ .

Some details

- Smoothing splines avoid the knot-selection issue, leaving a single λ to be chosen.
- The algorithmic details are too complex to describe here. In R, the function `smooth.spline()` will fit a smoothing spline.