

Moving Beyond Linearity

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When its not ...

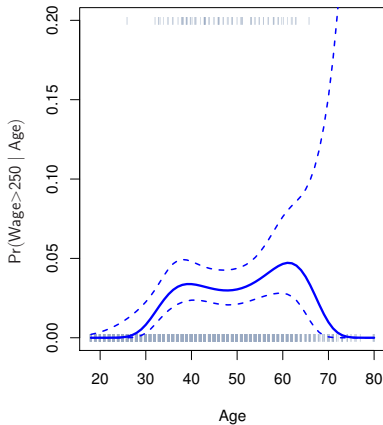
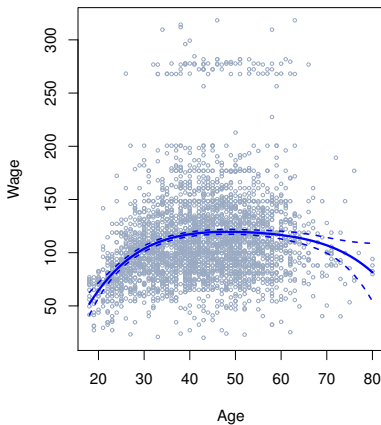
- polynomials,
- step functions,
- splines,
- local regression, and
- generalized additive models

offer a lot of flexibility, without losing the ease and interpretability of linear models.

Polynomial Regression

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \dots + \beta_d x_i^d + \epsilon_i$$

Degree-4 Polynomial



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- Since $\hat{f}(x_0)$ is a linear function of the $\hat{\beta}_\ell$, can get a simple expression for *pointwise-variances* $\text{Var}[\hat{f}(x_0)]$ at any value x_0 . In the figure we have computed the fit and pointwise standard errors on a grid of values for x_0 . We show $\hat{f}(x_0) \pm 2 \cdot \text{se}[\hat{f}(x_0)]$.

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- We either fix the degree d at some reasonably low value, else use cross-validation to choose d .

Details continued

- Logistic regression follows naturally. For example, in figure we model

$$\Pr(y_i > 250|x_i) = \frac{\exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \dots + \beta_d x_i^d)}{1 + \exp(\beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \dots + \beta_d x_i^d)}.$$

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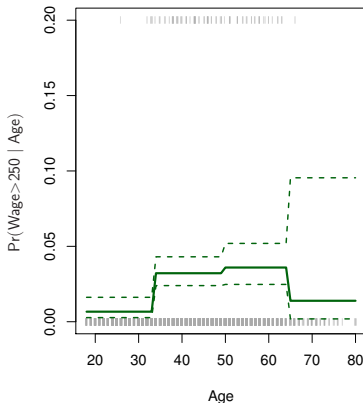
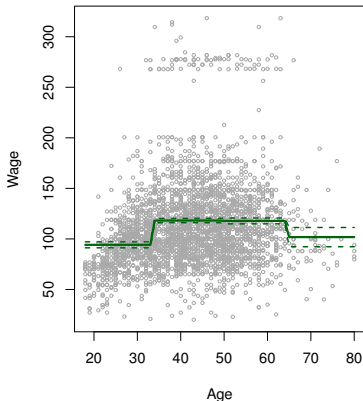
- To get confidence intervals, compute upper and lower bounds on *on the logit scale*, and then invert to get on probability scale.
- Can do separately on several variables—just stack the variables into one matrix, and separate out the pieces afterwards (see GAMs later).
- Caveat: polynomials have notorious tail behavior — very bad for extrapolation.
- Can fit using $\mathbf{y} \sim \text{poly}(\mathbf{x}, \text{degree} = 3)$ in formula.

Step Functions

Another way of creating transformations of a variable — cut the variable into distinct regions.

$$C_1(X) = I(X < 35), \quad C_2(X) = I(35 \leq X < 65), \dots, C_3(X) = I(X \geq 65)$$

Piecewise Constant



Step functions continued

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- In R: `I(year < 2005)` or `cut(age, c(18, 25, 40, 65, 90))`.
- Choice of cutpoints or *knots* can be problematic. For creating nonlinearities, smoother alternatives such as *splines* are available.

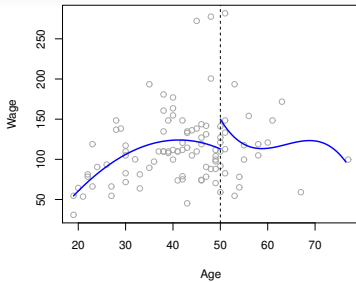
Piecewise Polynomials

- Instead of a single polynomial in X over its whole domain, we can rather use different polynomials in regions defined by knots. E.g. (see figure)

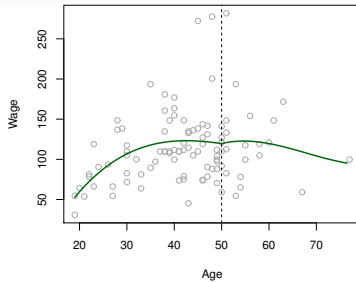
$$y_i = \begin{cases} \beta_{01} + \beta_{11}x_i + \beta_{21}x_i^2 + \beta_{31}x_i^3 + \epsilon_i & \text{if } x_i < c; \\ \beta_{02} + \beta_{12}x_i + \beta_{22}x_i^2 + \beta_{32}x_i^3 + \epsilon_i & \text{if } x_i \geq c. \end{cases}$$

- Better to add constraints to the polynomials, e.g. continuity.
- *Splines* have the “maximum” amount of continuity.

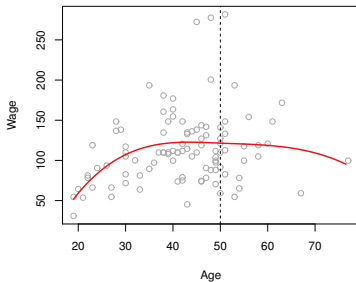
Piecewise Cubic



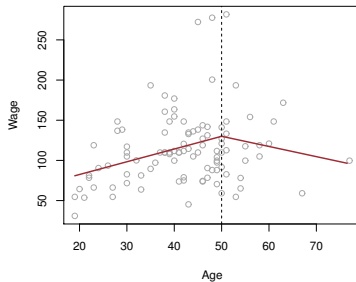
Continuous Piecewise Cubic



Cubic Spline



Linear Spline



Linear Splines

A linear spline with knots at ξ_k , $k = 1, \dots, K$ is a piecewise linear polynomial continuous at each knot.

We can represent this model as

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_{K+1} b_{K+1}(x_i) + \epsilon_i,$$

where the b_k are *basis functions*.

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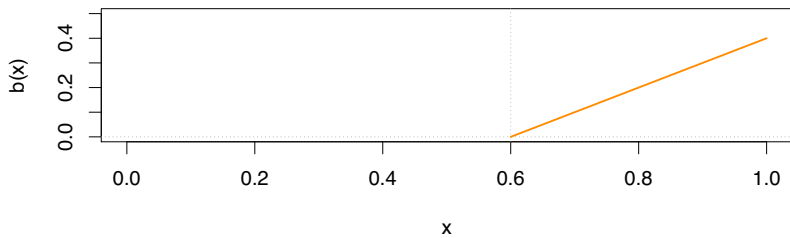
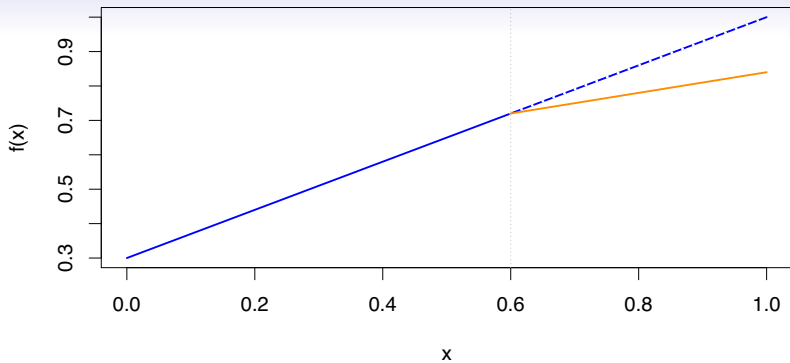
$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_{K+1} b_{K+1}(x_i) + \epsilon_i,$$

where the b_k are *basis functions*.

$$\begin{aligned} b_1(x_i) &= x_i \\ b_{k+1}(x_i) &= (x_i - \xi_k)_+, \quad k = 1, \dots, K \end{aligned}$$

Here the $()_+$ means *positive part*, i.e.

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



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

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

$$b_1(x_i) = x_i$$

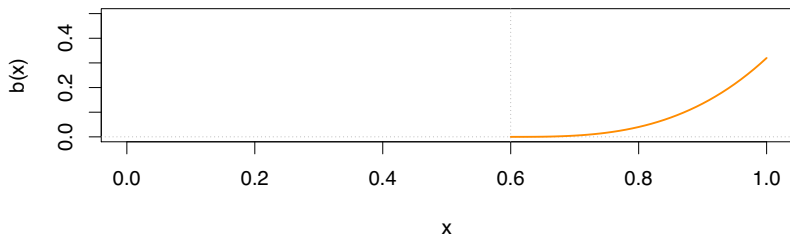
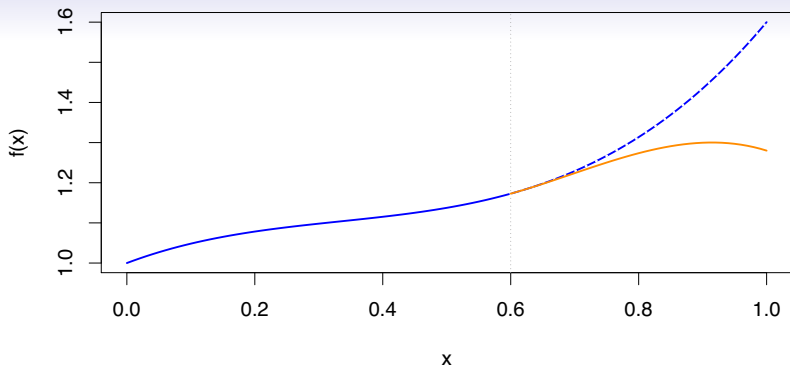
$$b_2(x_i) = x_i^2$$

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

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

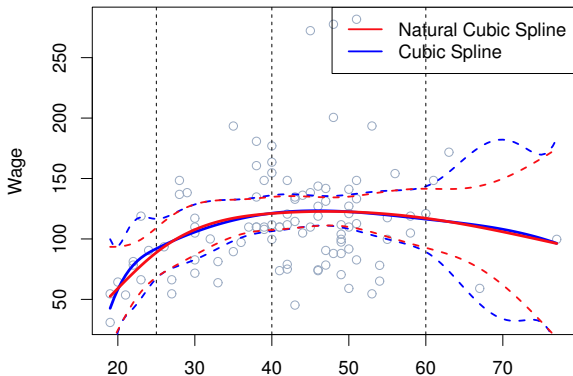
where

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



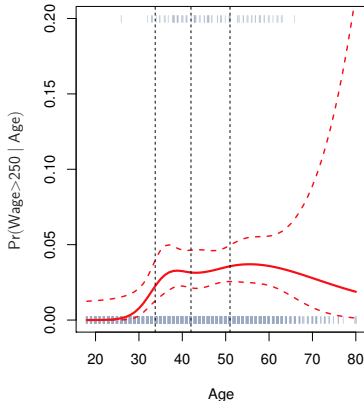
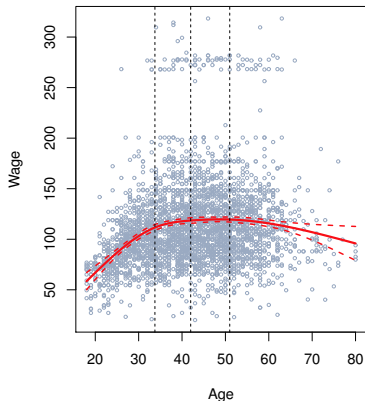
Natural Cubic Splines

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.



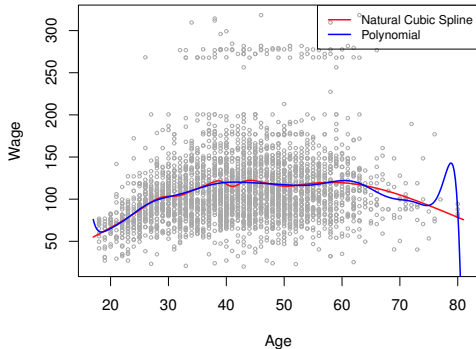
Fitting splines in R is easy: `bs(x, ...)` for any degree splines, and `ns(x, ...)` for natural cubic splines, in package `splines`.

Natural Cubic Spline



Knot placement

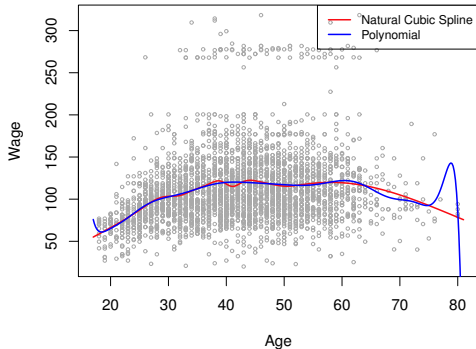
- One strategy is to decide K , the number of knots, and then place them at appropriate quantiles of the observed X .
- A cubic spline with K knots has $K + 4$ parameters or degrees of freedom.
- A natural spline with K knots has K degrees of freedom.



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

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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:

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

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 - 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.

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- The algorithmic details are too complex to describe here. In R, the function `smooth.spline()` will fit a smoothing spline.
- The vector of n fitted values can be written as $\hat{\mathbf{g}}_\lambda = \mathbf{S}_\lambda \mathbf{y}$, where \mathbf{S}_λ is a $n \times n$ matrix (determined by the x_i and λ).
- The *effective degrees of freedom* are given by

$$df_\lambda = \sum_{i=1}^n \{\mathbf{S}_\lambda\}_{ii}.$$

Smoothing Splines continued — choosing λ

- We can specify df rather than λ !

In R: `smooth.spline(age, wage, df = 10)`

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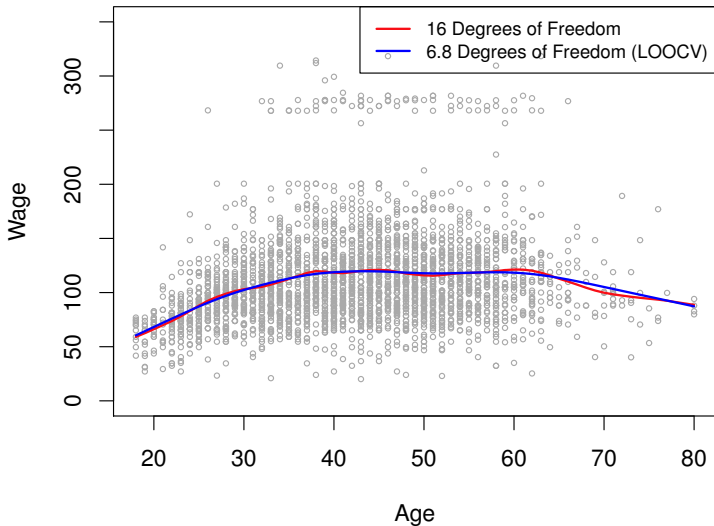
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- The leave-one-out (LOO) cross-validated error is given by

$$\text{RSS}_{cv}(\lambda) = \sum_{i=1}^n (y_i - \hat{g}_{\lambda}^{(-i)}(x_i))^2 = \sum_{i=1}^n \left[\frac{y_i - \hat{g}_{\lambda}(x_i)}{1 - \{\mathbf{S}_{\lambda}\}_{ii}} \right]^2.$$

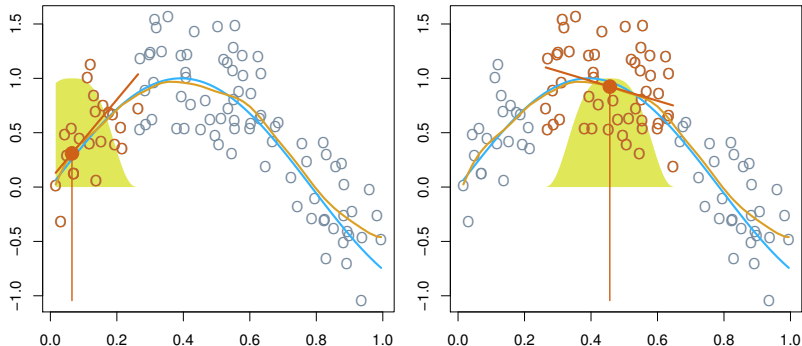
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Smoothing Spline



Local Regression

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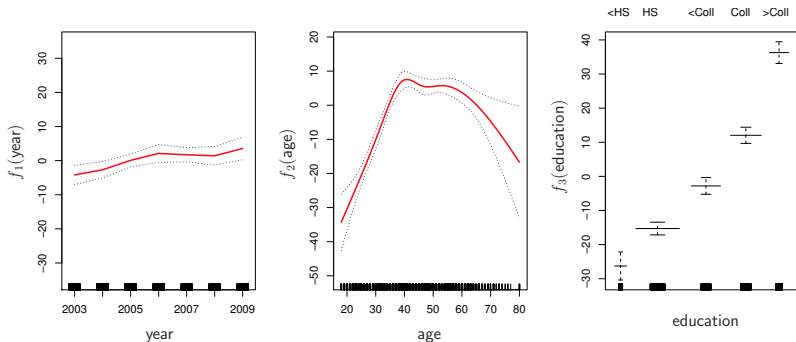
With a sliding weight function, we fit separate linear fits over the range of X by weighted least squares.

See text for more details, and `loess()` function in R.

Generalized Additive Models

Allows for flexible nonlinearities in several variables, but retains the additive structure of linear models.

$$y_i = \beta_0 + f_1(x_{i1}) + f_2(x_{i2}) + \cdots + f_p(x_{ip}) + \epsilon_i.$$



GAM details

- Can fit a GAM simply using, e.g. natural splines:

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lm(wage ~ ns(year, df = 5) + ns(age, df = 5) + education)
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- Can use smoothing splines or local regression as well:

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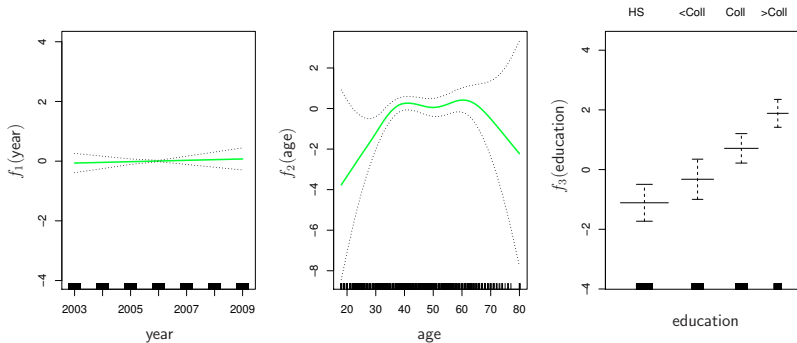
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- GAMs are additive, although low-order interactions can be included in a natural way using, e.g. bivariate smoothers or interactions of the form `ns(age, df=5):ns(year, df=5)`.

GAMs for classification

$$\log \left(\frac{p(X)}{1 - p(X)} \right) = \beta_0 + f_1(X_1) + f_2(X_2) + \cdots + f_p(X_p).$$



```
gam(I(wage > 250) ~ year + s(age, df = 5) + education, family = binomial)
```