Statistical Machine Learning

Moving Beyond Linearity

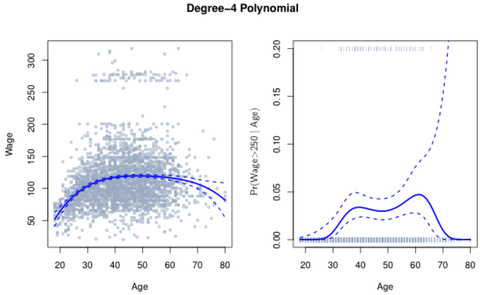
Moving Beyond Linearity

- The truth is never linear! Or almost never!
- But often the linearity assumption is good enough.
- 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

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \ldots + \beta_d x_i^d + \varepsilon_i$$

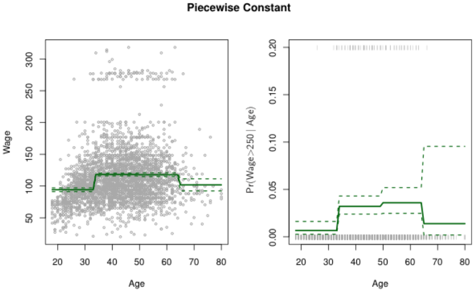


Can fit using `y` $\sim$ `poly(x, degree = 3)` in formula.

Step Functions

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

$$C_1(X) = I(X < 35), C_2(X) = I(35 \leq x < 50), \ldots, C_k = I(X > 65)$$

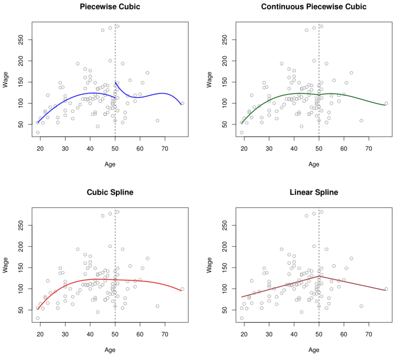


Step Functions (cont.)

- Easy to work with. Creates a series of dummy variables representing each group.
- In R: `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.

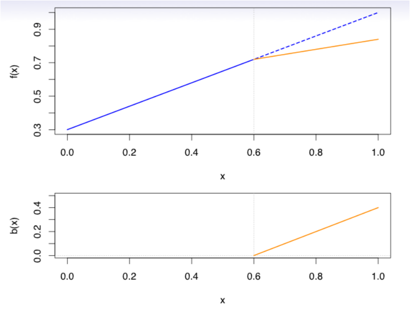
Piecewise Polynomials

- 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)
- Better to add constraints to the polynomials, e.g. continuity, differentiability.
- Splines have the "maximum" amount of continuity.



Linear Splines

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



Linear Splines: Details

- We can represent this model as

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \ldots + + \beta_{K+1} b_{K+1}(x_i) + \varepsilon$$

$ where the b_k are basis functions.

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

- Here $(\cdot)_+$ means positive part, i.e.

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

Cubic Splines

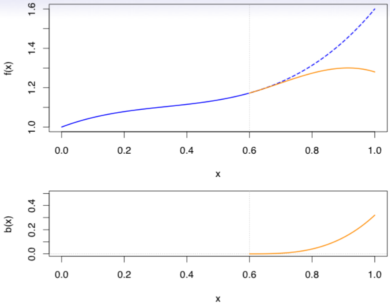
- A cubic spline with knots at $\xi_k, k = 1, \ldots, K$ is a piecewise cubic polynomial continuous second derivatives at each knot.
- Again we can represent this model with truncated power basis functions

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \ldots + + \beta_{K+3} b_{K+1}(x_i) + \varepsilon$$

where

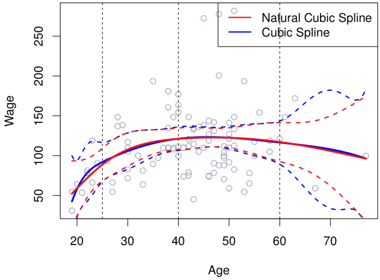
$$\begin{aligned} b_1(x) &= x \\ b_2(x) &= x^2 \\ b_3(x) &= x^3 \\ b_{k+3}(x) &= (x - \xi_k)_+^3, \quad k = 1, \ldots, K \end{aligned}$$

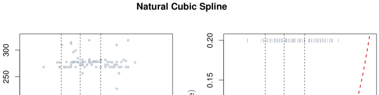
Cubic Splines (cont)



Natural Cubic Splines

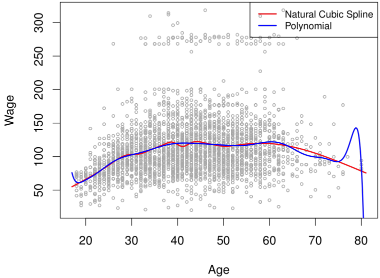
- A natural cubic spline extrapolates linearly beyond the boundary knots.
- This adds $4 = 2 \times 2$ extra constraints, and allows us to put more internal knots for the same degrees of freedom as a regular cubic spline.





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 15 df

Splines with Penalty

- Fixed df splines are useful tools, but are not truly nonparametric
- Choices regarding the number of knots and where they are located are fundamentally parametric choices and have a large effect on the fit
- Furthermore, assuming that you place knots at quantiles, models will not be nested inside each other, which complicates hypothesis testing
  - P-Spline: We have the same spline model with a much denser grid of knots. The estimates are obtained from ridge or lasso regression.
  - Smoothing Spline: We can avoid the knot selection problem altogether via the nonparametric formulation introduced at the beginning of lecture: choose the function g that minimizes

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

Smoothing Splines

- Consider this criterion for fitting a smooth function $g(\cdot)$

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

- 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 $\lambda \to \infty$, the function s 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 avoid the knot-selection issue, leaving a single λ to be chosen.
- In R, the function `smooth.spline()` will fit a smoothing spline
- The vector of n fitted values can be written as

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

  where S_λ is a $n \times n$ matrix (depends on x_i and λ)
- The effective degrees of freedom are given by $\text{trace}(S_\lambda)$

Choosing λ

- We can specify df rather than λ!
- In R: `smooth.spline(age, wage, df = 10)`
- The leave-one-out (LOO) cross-validated error is given by

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

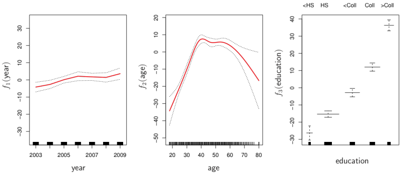
- In R: `smooth.spline(age, wage, cv = TRUE)`

Generalized additive function

A natural way to extend the multiple linear regression model is

$$y_i = \beta_0 + \beta_1 f(x_{i1}) + \ldots + + \beta_p f(x_{ip}) + \varepsilon$$

Take, for example, natural splines, and consider the task of fitting the model wage $= \beta_0 + f_1(\text{year}) + f_2(\text{age}) + f_3(\text{education}) + \varepsilon$



Pros and Cons of GAMs

Pros:

- GAMs allow us to fit a non-linear f_j to each X_j, so that we can automatically model non-linear relationships that standard linear regression will miss. This means that we do not need to manually try out many different transformations on each variable individually.
- The non-linear fits can potentially make more accurate predictions for the response Y.
- Because the model is additive, we can still examine the effect of each X_j on Y individually while holding all of the other variables fixed. Hence if we are interested in inference, GAMs provide a useful representation.
- The smoothness of the function f_j for the variable X_j can be summarized via degrees of freedom.

Cons:

- The main limitation of GAMs is that the model is restricted to be additive.