Moving Beyond Linearity

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See board for distinction between linear regression & linear models

- C1(x), C2(x), ... Cd(x) are basis functions for linear model

The truth is never linear!
Or almost never!

But often the linearity assumption is good enough.

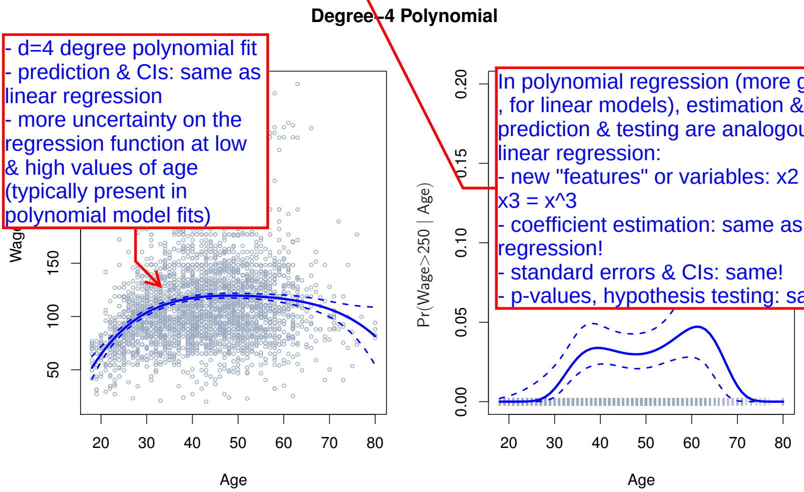
When its not ...

- 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

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

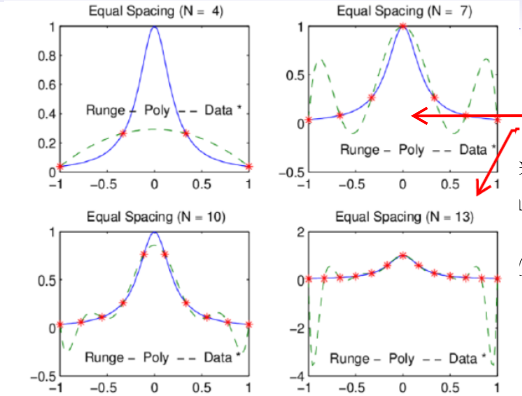


- d=4 degree polynomial fit
- prediction & CIs: same as linear regression
- more uncertainty on the regression function at low & high values of age (typically present in polynomial model fits)

In polynomial regression (more generally, for linear models), estimation & prediction & testing are analogous from linear regression:
- new "features" or variables: x2 = x^2, x3 = x^3
- coefficient estimation: same as linear regression!
- standard errors & CIs: same!
- p-values, hypothesis testing: same!

Details

- Create new variables $X_1 = X$, $X_2 = X^2$, etc and then treat as multiple linear regression.



Runge's phenomenon:
- for certain non-polynomial regression functions, fitting a higher-order polynomial can in fact give poor (highly oscillatory) predictions near domain boundaries
- why? higher-order polynomials are highly volatile - they capture global trends, but cannot capture well local trends.
- this is the key danger of polynomial modeling

X_2

$\hat{\beta}_2 x_0^2 + \hat{\beta}_3 x_0^3 + \hat{\beta}_4 x_0^4.$

Details

- Create new variables $X_1 = X$, $X_2 = X^2$, etc and then treat as multiple linear regression.
- Not really interested in the coefficients; more interested in the fitted function values at any value x_0:

$$\hat{f}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0 + \hat{\beta}_2 x_0^2 + \hat{\beta}_3 x_0^3 + \hat{\beta}_4 x_0^4.$$

- Since $\hat{f}(x_0)$ is a linear function of the $\hat{\beta}_\ell$, can get a simple expression for *pointwise-variances* $\mathrm{Var}[\hat{f}(x_0)]$ 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 $\hat{f}(x_0) \pm 2 \cdot \mathrm{se}[\hat{f}(x_0)]$.

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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

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

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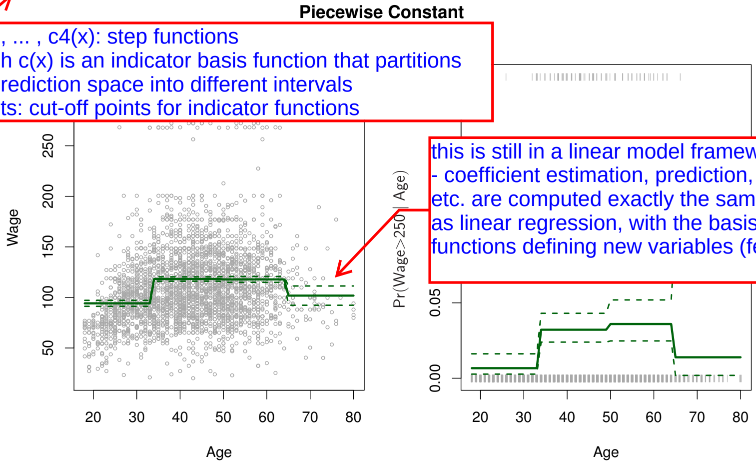
- To get confidence intervals, compute upper and lower bounds on *on the logit scale*, and then invert to get on probability scale.
- Can do separately on several variables—just stack the variables into one matrix, and separate out the pieces afterwards (see GAMs later).
- Caveat: polynomials have notorious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

Step Functions

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

$$C_1(X) = I(X < 35), \quad C_2(X) = I(35 \leq X < 50), \ldots, C_3(X) = I(X \geq 65)$$

c1(x), ... , c4(x): step functions
- each c(x) is an indicator basis function that partitions the prediction space into different intervals
- knots: cut-off points for indicator functions



this is still in a linear model framework:
- coefficient estimation, prediction, CIs, etc. are computed exactly the same way as linear regression, with the basis functions defining new variables (features)

Step functions continued

- Easy to work with. Creates a series of dummy variables representing each group.

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- Useful way of creating interactions that are easy to interpret. For example, interaction effect of `Year` and `Age`:

$$I(\texttt{Year} < 2005) \cdot \texttt{Age}, \quad I(\texttt{Year} \geq 2005) \cdot \texttt{Age}$$

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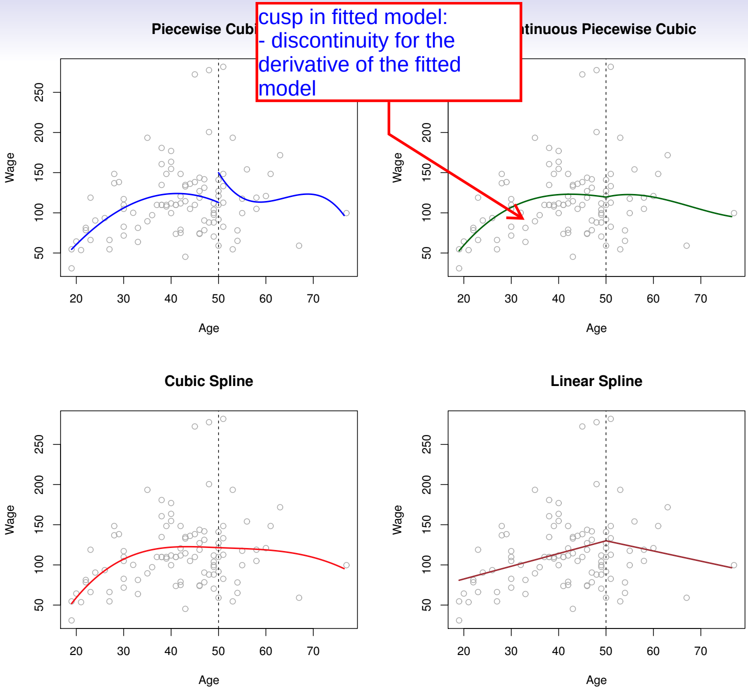
  would allow for different linear functions in each age category.
- In R: `I(year < 2005)` or `cut(age, c(18, 25, 40, 65, 90))`.
- Choice of cutpoints or *knots* can be problematic. For creating nonlinearities, smoother alternatives such as *splines* are available.

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
cusp in fitted model:
- discontinuity for the derivative of the fitted model
Cubic Spline
Linear Spline
Wage
Age
20
30
40
50
60
70
50
100
150
200
250

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

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

where the b_k are *basis functions*.

Claim: linear splines can be represented as the following linear model:

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typo: K+1 basis functions

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where the b_k are *basis functions*.

baseline linear function

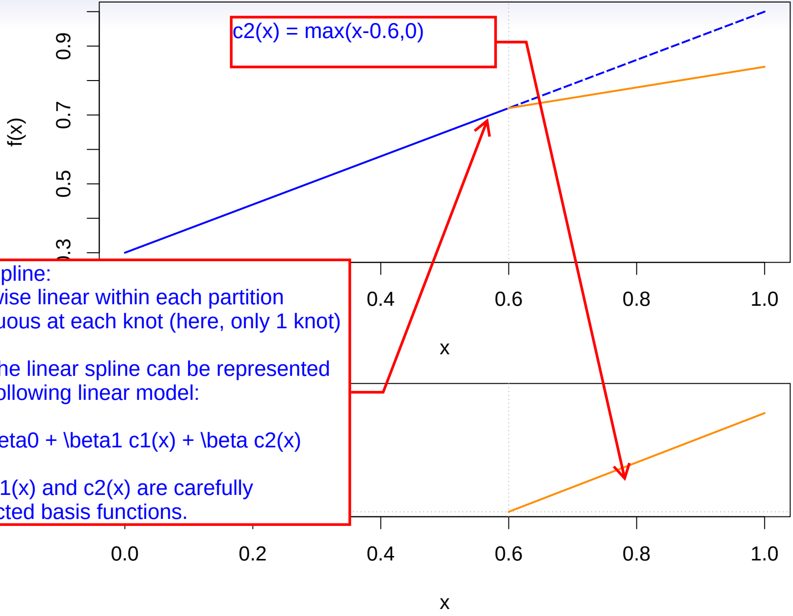
$$\begin{aligned} b_1(x_i) &= x_i \\ b_{k+1}(x_i) &= (x_i - \xi_k)_+, \quad k \end{aligned}$$

allows for linear flexibility after knot \xi_k

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

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

this then becomes a linear model:
- coefficient estimation, standard errors, CIs, hypothesis testing: same as for linear regression



Linear spline:
- piecewise linear within each partition
- continuous at each knot (here, only 1 knot)

Claim: the linear spline can be represented by the following linear model:

f(x) = \beta0 + \beta1 c1(x) + \beta c2(x)

where c1(x) and c2(x) are carefully constructed basis functions.

degrees-of-freedom (df): "the number of model parameters to fit". we'll generalize this later for non-integer df.
- model df can be thought of as a proxy for model complexity

- cubic splines with K knots will have K+4 dfs
- linear splines with K knots will have K+2 dfs
- adding additional constraints reduces the number of dfs

...bic Splines

... $\xi_k,\ k = 1, \ldots, K$ *is a piecewise*

...*nuou*... *rder 2 at*

why can we not make this order 3? it would then be the same cubic function over different partitions - we lose our local modeling property!

mo... ower basis

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

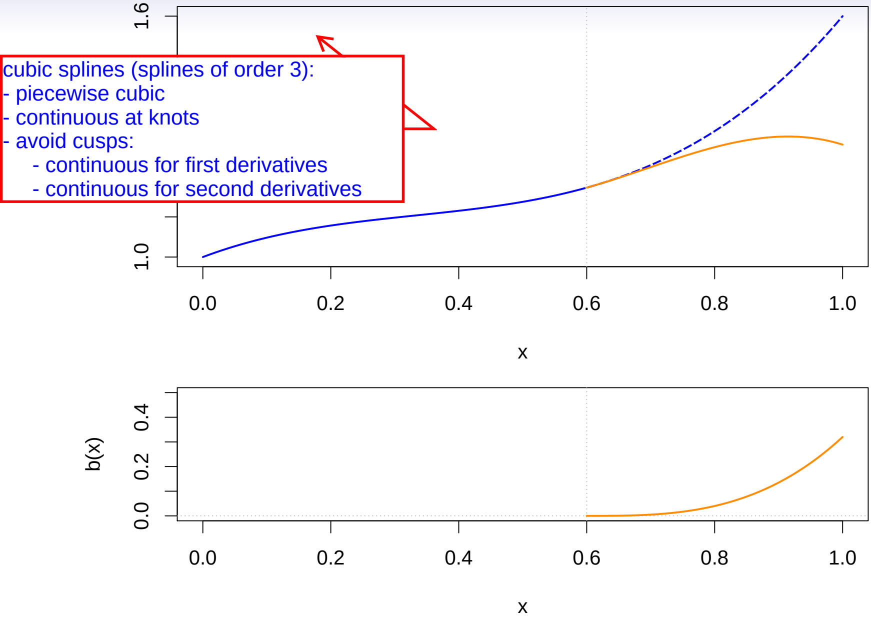
Claim: a cubic spline can be represented as the following linear model
- efficient coefficient estimation, standard errors, CIs, testing: same as what we did in linear regression

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

baseline cubic function

where

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


cubic splines (splines of order 3):
- piecewise cubic
- continuous at knots
- avoid cusps:
- continuous for first derivatives
- continuous for second derivatives
1.6
1.0
0.0
0.2
0.4
0.6
0.8
1.0
x
b(x)
0.0
0.2
0.4
0.0
0.2
0.4
0.6
0.8
1.0
x

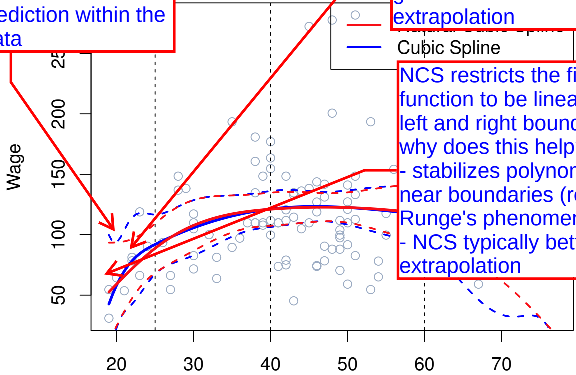
Natural Cubic

NCS with K knots => K dfs
(K+4) - 4 constraints (2 on each side)

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.

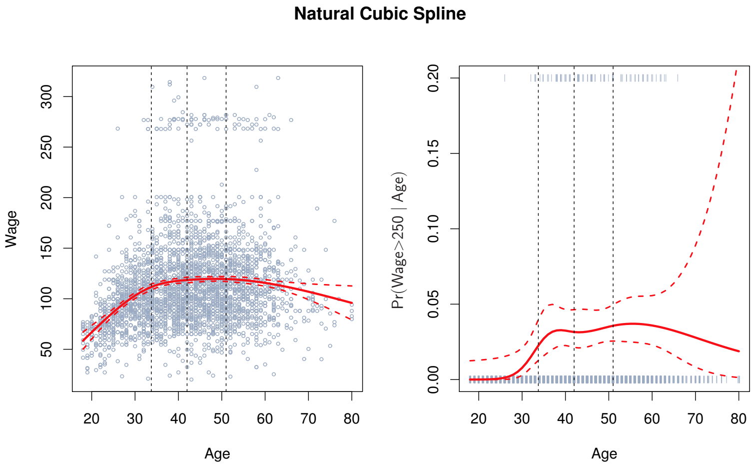
limitation of CS: it can be quite volatile near prediction edges, so it's not good / stable for extrapolation

extrapolate: prediction beyond the range of your data
interpolation: prediction within the range of your data



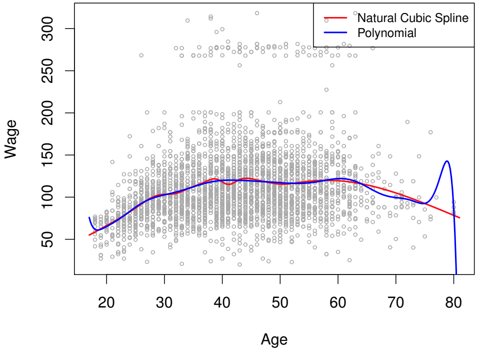
NCS restricts the fitted function to be linear at the left and right boundaries.
why does this help?
- stabilizes polynomial fits near boundaries (recall Runge's phenomenon)
- NCS typically better for extrapolation

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



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

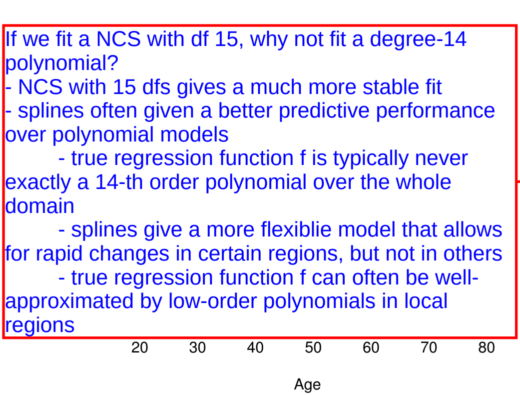
What are different ways to vary the bias-variance trade-off for splines?
- changing the number of knots K
- changing the degree of polynomials within each partition (linear splines, cubic splines, etc.)
- regularization (shrinkage) on the linear model representation of splines

…ntiles of the observed X.

…as $K + 4$ parameters or

… has K degrees of freedom.

If we fit a NCS with df 15, why not fit a degree-14 polynomial?
- NCS with 15 dfs gives a much more stable fit
- splines often given a better predictive performance over polynomial models
    - true regression function f is typically never exactly a 14-th order polynomial over the whole domain
    - splines give a more flexiblie model that allows for rapid changes in certain regions, but not in others
    - true regression function f can often be well-approximated by low-order polynomials in local regions

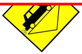


Comparison of a degree-14 polynomial and a natural cubic spline, each with 15df.

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

Smoothing Sp

why smoothing splines?
- regularization (shrinkage) can help in estimating coefficients from linear models
- the choice of knot selection can also be subjective

This section is a little bit mathematical 

Consider this criterion for fitting a smooth function $g(x)$ to s

"RSS term": measures training error

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

penalty term:
- penalizes a measure of the smoothness of a function
- the penalty equals 0 when the function g is linear
- the penalty becomes large if the function is very wiggly

Smoothing Splines

This section is a little bit mathematical 

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

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  - The smaller λ, the more wiggly the function, eventually interpolating y_i when $\lambda = 0$.
  - As $\lambda \to \infty$, 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.

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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 $\mathbf{S}_\lambda$ 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)`

Smoothing Splines continued — choosing λ

- We can specify *df* rather than λ!

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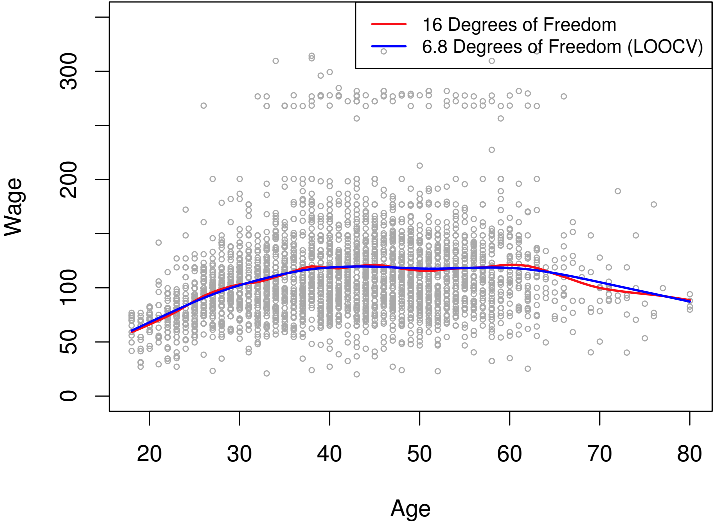
- The leave-one-out (LOO) cross-validated error is given by

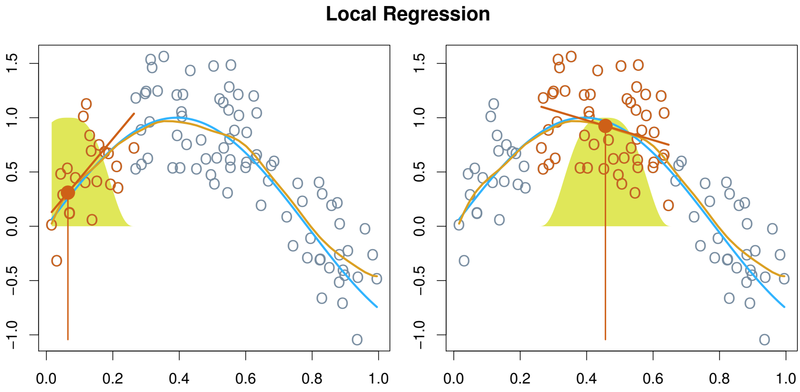
$$\mathrm{RSS}_{cv}(\lambda) = \sum_{i=1}^{n} (y_i - \hat{g}_\lambda^{(-i)}(x_i))^2 = \sum_{i=1}^{n} \left[\frac{y_i - \hat{g}_\lambda(x_i)}{1 - \{\mathbf{S}_\lambda\}_{ii}} \right]^2.$$

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

Smoothing Spline



Local Regression



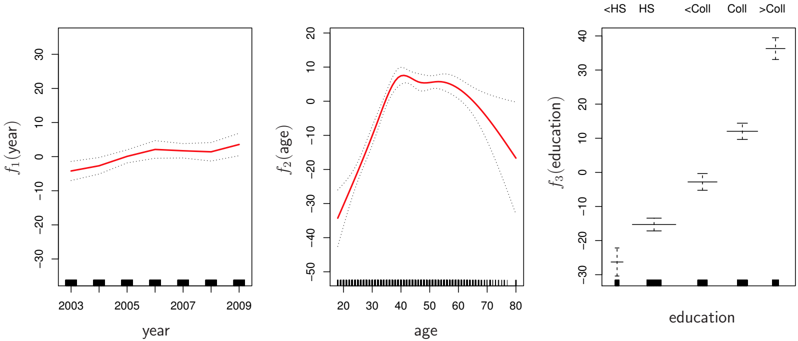
With a sliding weight function, we fit separate linear fits over the range of X by weighted least squares.

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:

  $\texttt{lm}(\texttt{wage} \sim \texttt{ns}(\texttt{year}, \texttt{df} = 5) + \texttt{ns}(\texttt{age}, \texttt{df} = 5) + \texttt{education})$

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- Can mix terms — some linear, some nonlinear — and use `anova()` to compare models.
- Can use smoothing splines or local regression as well:

  $$\texttt{gam}(\texttt{wage} \sim \texttt{s}(\texttt{year}, \texttt{df} = 5) + \texttt{lo}(\texttt{age}, \texttt{span} = .5) + \texttt{education})$$

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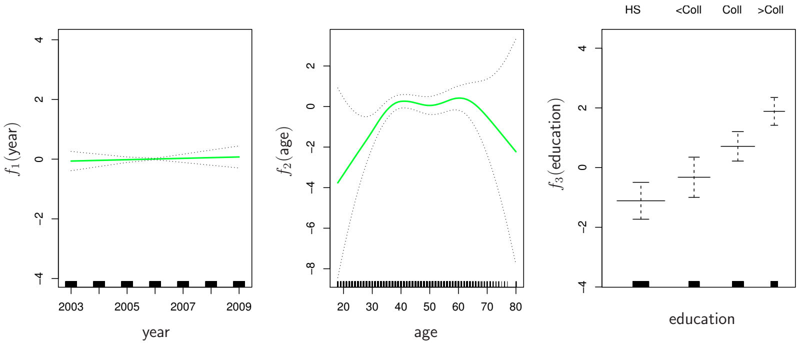
- Can mix terms — some linear, some nonlinear — and use `anova()` to compare models.
- Can use smoothing splines or local regression as well:

  `gam(wage ~ s(year, df = 5) + lo(age, span = .5) + education)`

- 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

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



$\texttt{gam(I(wage} > \texttt{250)} \sim \texttt{year} + \texttt{s(age, df} = \texttt{5)} + \texttt{education, family} = \texttt{binomial)}$