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When its not . . .

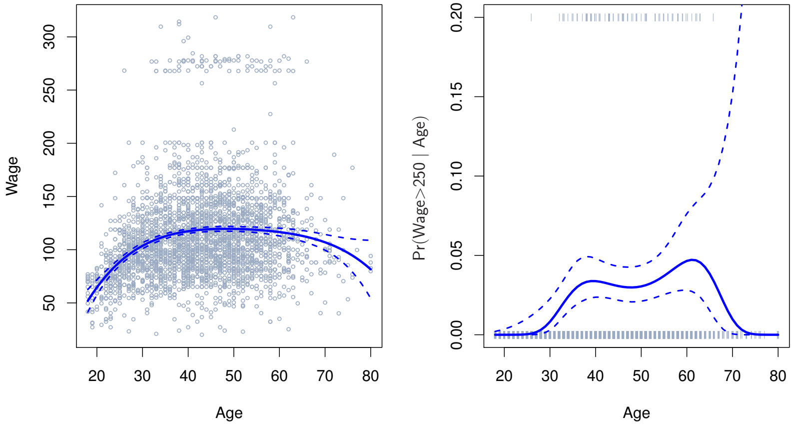
- polynomials,
- step functions,
- splines,
- local regression, and
- generalized additive models

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

Polynomial Regression

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

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* $\mathrm{Var}[\hat{f}(x_0)]$ 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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```
x' = (1,x0,x0^2,x0^3,x0^4). fhat = x'*betahat
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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

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

- To get confidence intervals, compute upper and lower bounds on *on the logit scale*, and then invert to get on probability scale.

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=> this gives the CI for logit(p(x0)); then apply "expit" (=logit^(-1)) to both sides

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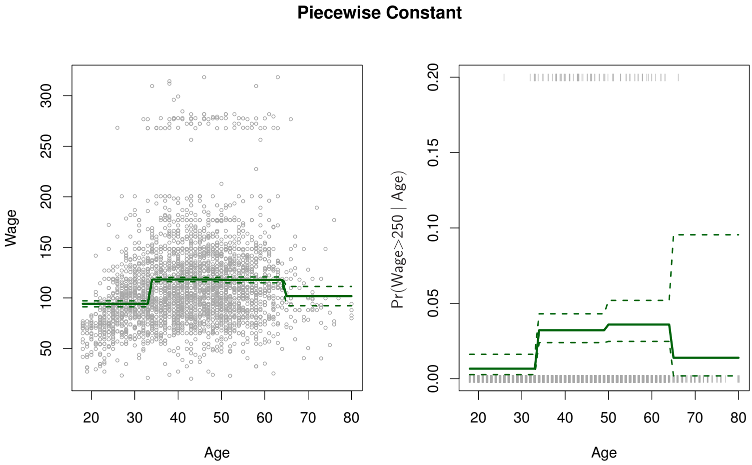
- To get confidence intervals, compute upper and lower bounds on *on the logit scale*, and then invert to get on probability scale.
- Can do separately on several variables—just stack the variables into one matrix, and separate out the pieces afterwards (see GAMs later).
- Caveat: polynomials have notorious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

Step Functions

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

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



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

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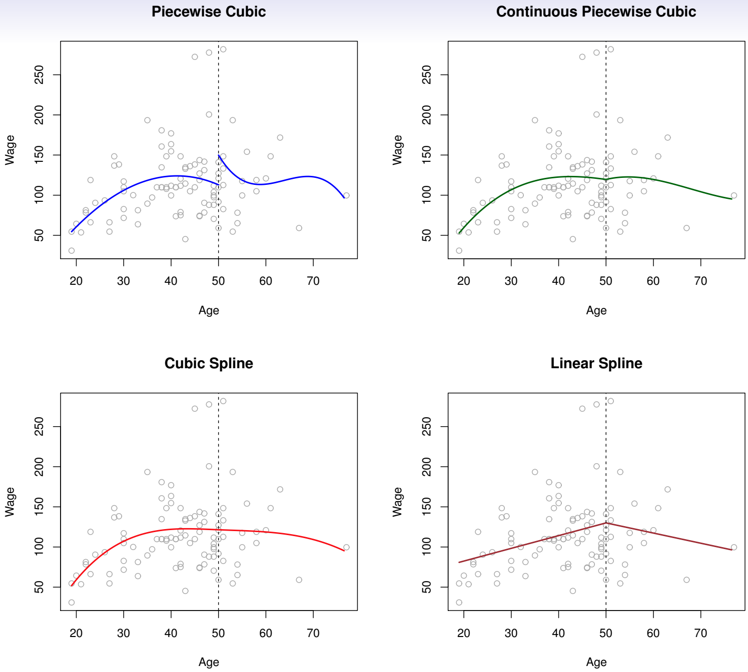
- In R: `I(year < 2005)` or `cut(age, c(18, 25, 40, 65, 90))`.
- Choice of cutpoints or *knots* can be problematic. For creating nonlinearities, smoother alternatives such as *splines* are available.

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

Linear Splines

A linear spline with knots at ξ_k, $k = 1, \ldots, K$ *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*.

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where the b_k are *basis functions*.

K+1 rather than K+3

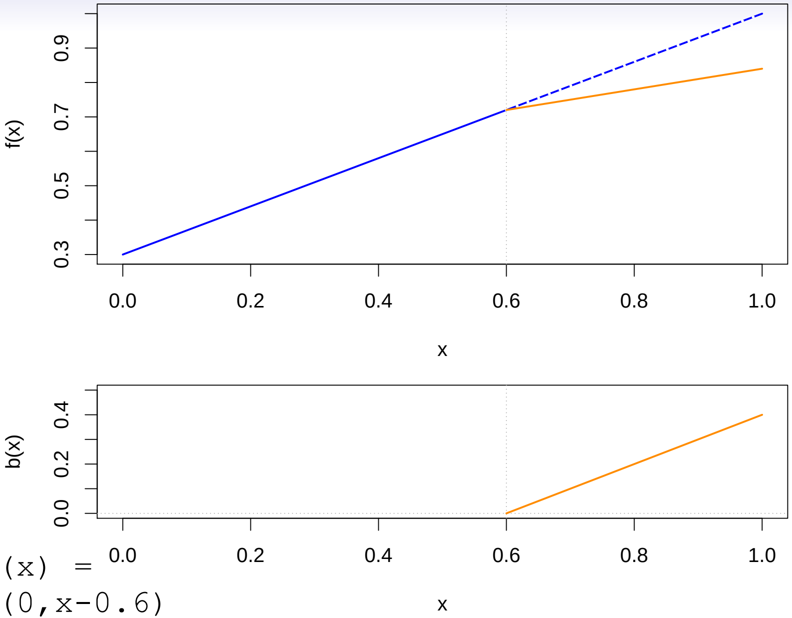
$$\begin{aligned} b_1(x_i) &= x_i \\ b_{k+1}(x_i) &= (x_i - \xi_k)_+, \quad k = 1, \ldots, K \end{aligned}$$

= max(0, x_i - xi_k)

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

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

`1* b_1(x) - 0.5*b_2(x)`



`b_2(x) = max(0,x-0.6)`

Cubic Splines

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

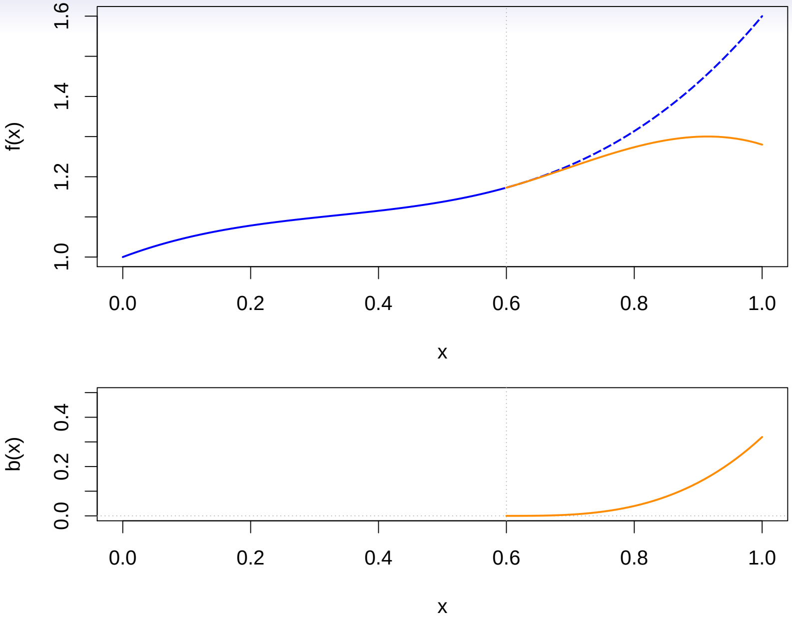
Again we can represent this model with truncated power basis functions

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

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

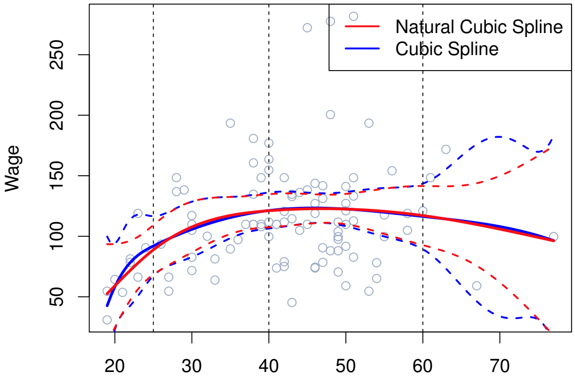
where

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

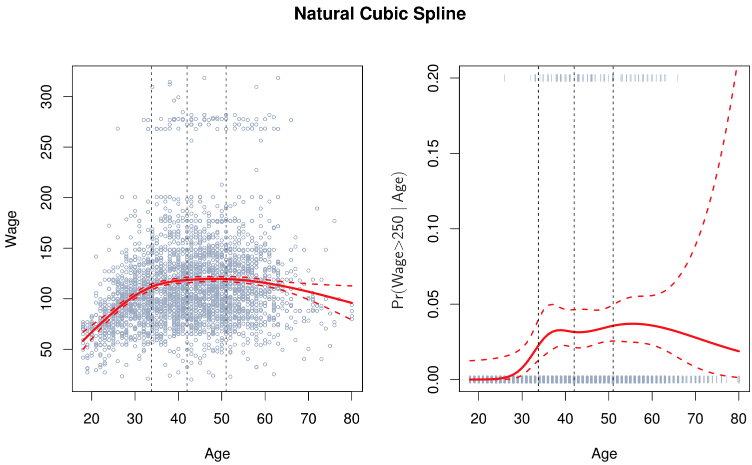

f(x)
1.0
1.2
1.4
1.6
0.0
0.2
0.4
0.6
0.8
1.0
x
b(x)
0.0
0.2
0.4
0.0
0.2
0.4
0.6
0.8
1.0
x

Natural Cubic 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.

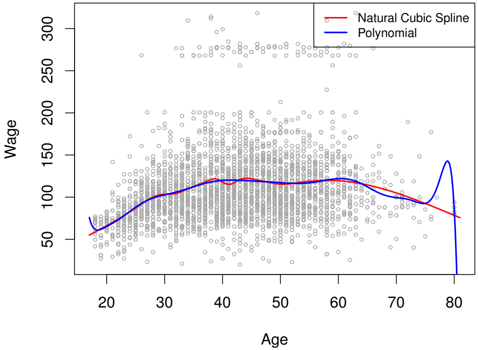


Fitting splines in R is easy: `bs(x, ...)` for any degree splines, and `ns(x, ...)` for natural cubic splines, in package `splines`.



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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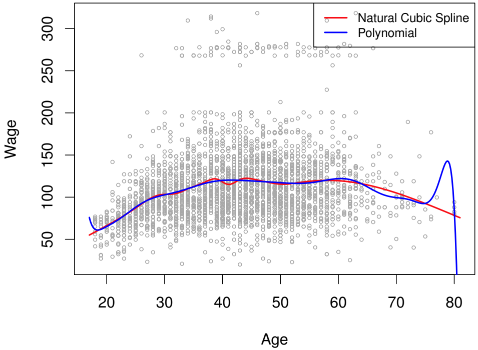

Comparison of a degree-14 polynomial and a natural cubic spline, each with 15df.

`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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  - As $\lambda \to \infty$, the function $g(x)$ becomes linear.

Smoothing Splines continued

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- 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.
- 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)`

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

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

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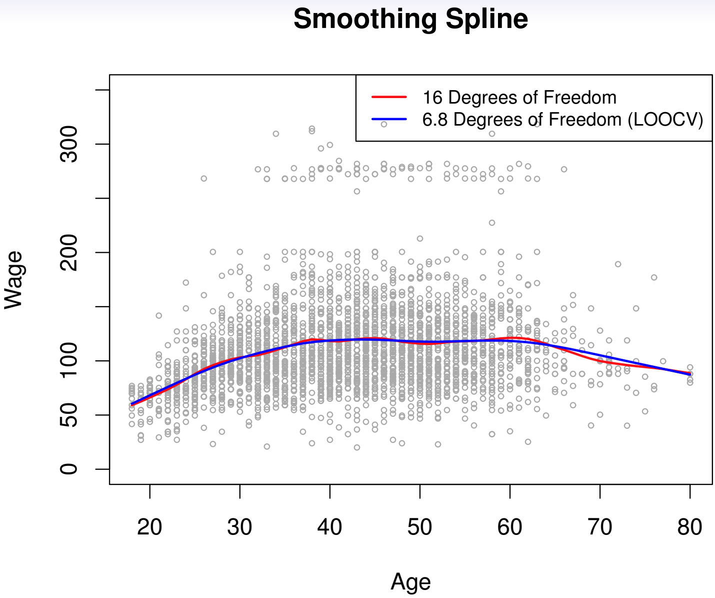
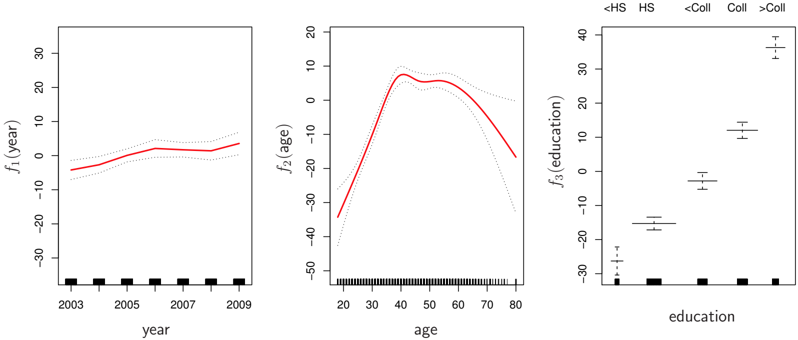

Smoothing Spline
16 Degrees of Freedom
6.8 Degrees of Freedom (LOOCV)
Wage
0
50
100
200
300
20
30
40
50
60
70
80
Age

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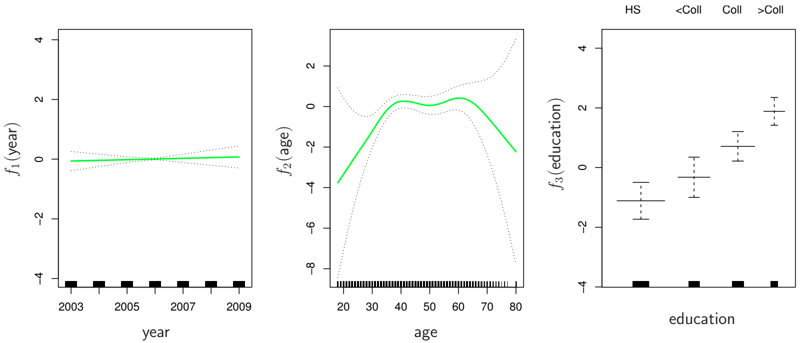
- GAMs are additive, although low-order interactions can be included in a natural way using, e.g. bivariate smoothers or interactions of the form `ns(age,df=5):ns(year,df=5)`.

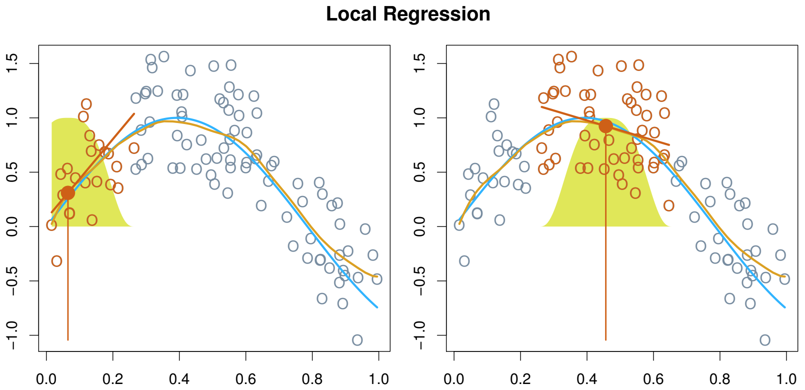
GAMs for classification

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



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

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.