BIG DATA ANALYTICS
Moving Beyond Linearity

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Step Functions

Regression Splines

Smoothing Splines

Local Regression

Generalized Additive Models

Linear models

- Linear models:
  - relatively simple to describe and implement
  - have advantages in terms of interpretation and inference
  - significant limitations in terms of predictive power:
    - the linearity assumption is almost always an approximation (sometimes a poor one)
- Relax the linearity assumption while still maintaining as much interpretability as possible:
  - polynomial regression
  - step functions
  - splines
  - local regression
  - generalized additive models

Extensions

- *Polynomial regression*:
  - extends the linear model by adding extra predictors X^2, X^3, ...
  - a simple way to provide a nonlinear fit to data
- *Step functions*:
  - cuts the range of a variable into K distinct regions
  - fits a piecewise constant function

Extensions

- *Regression splines*:
  - more flexible than polynomials and step functions
  - an extension of both
  - divides the range of X into K distinct regions
  - within each region, a polynomial function is fitted to the data
  - polynomials are constrained: they join smoothly at the region boundaries
  - can produce an extremely flexible fit

Extensions

- *Smoothing splines*:
  - similar to regression splines
  - result from minimizing a residual sum of squares criterion subject to a smoothness penalty
- *Local regression*:
  - similar to splines
  - the regions are allowed to overlap
- *Generalized additive models*: allow to extend the methods above to deal with multiple predictors.

Outline

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Step Functions

- Breaks the range of X into bins, and fits a different constant in each bin:
  - converting a continuous variable into an ordered categorical variable
  - we create cutpoints $c_1, c_2, ..., c_K$ in the range of X
  - construct $K + 1$ new variables:

$$
\begin{aligned}
C_0(X) &= I(X < c_1) \\
C_1(X) &= I(c_1 \leq X < c_2) \\
&\dots \\
C_K(X) &= I(c_K \leq X)
\end{aligned}
$$

  where $I(\cdot)$ is an indicator function

Step Functions

- $I(\cdot)$ returns a 1 if the condition is true, and returns a 0 otherwise
- For example, $I(c_K \leq X)$ equals 1 if $c_K \leq X$ and equals 0 otherwise
- Also called dummy variables
- For any value of X

$$C_0(X) + C_1(X) + ... + C_K(X) = 1$$

since X must be in exactly one of the $K + 1$ intervals

Step Functions

- We use least squares to fit a linear model using $C_1(X), C_2(X), ..., C_K(X)$ as predictors:

$$y_i = \beta_0 + \beta_1 C_1(x_i) + \beta_2 C_2(x_i) + \cdots + \beta_K C_K(x_i) + \epsilon_i$$

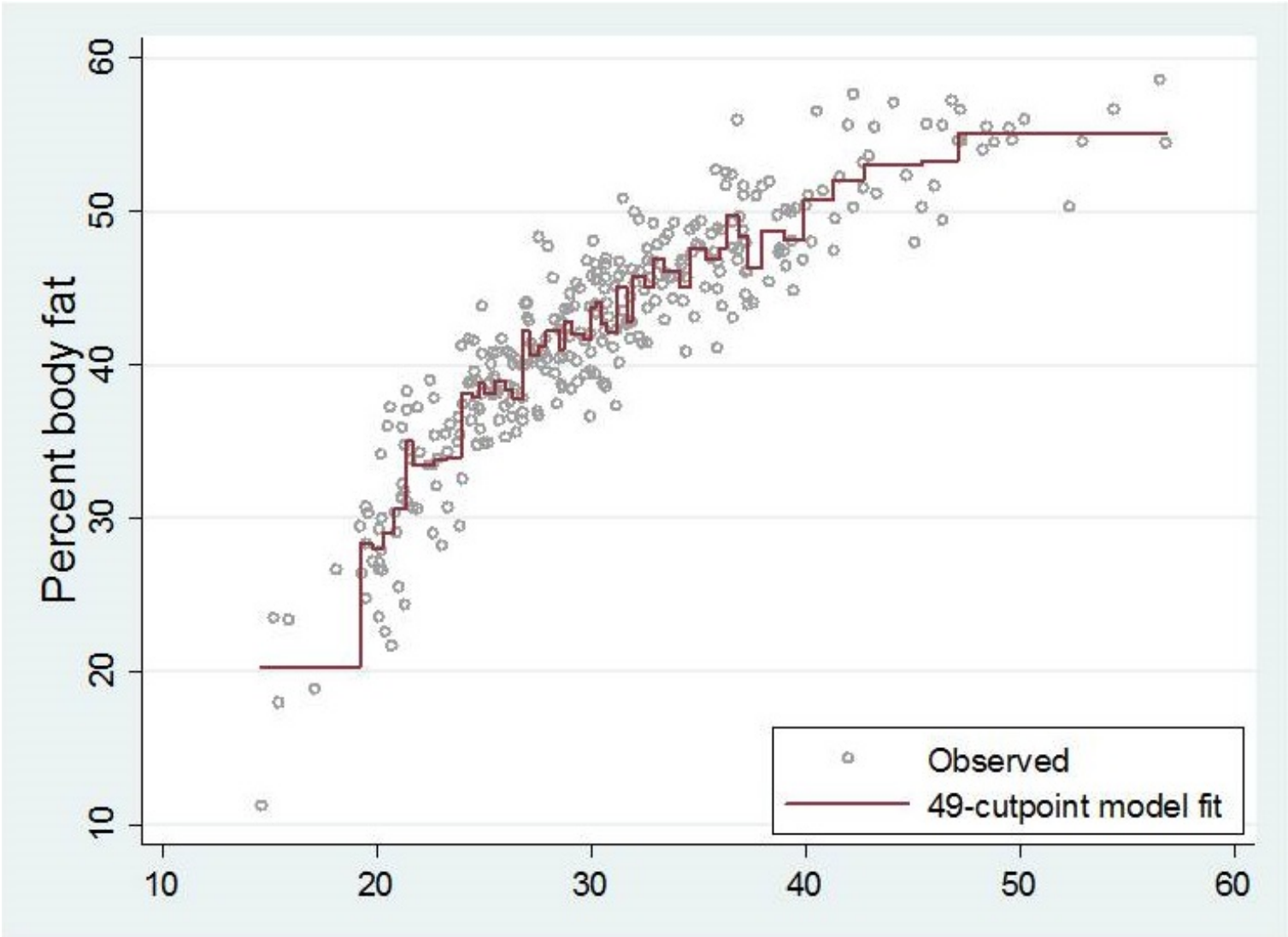
- For a given value of X, at most one of $C_1, C_2, ..., C_K$ can be non-zero
- When $X < c_1$, all of the predictors are zero $\implies$ β_0 is the mean value of Y for $X < c_1$
- For $c_j \leq X < c_{(j+1)}$ we get $\beta_0 + \beta_j \implies \beta_j$ is the average increase in the response for X in $c_j \leq X < c_{(j+1)}$ relative to $X < c_1$

Step Functions

$$y_i = \beta_0 + \beta_1 C_1(x_i) + \beta_2 C_2(x_i) + \cdots + \beta_K C_K(x_i) + \epsilon_i$$

- We exclude $C_0(X)$ as a predictor because it is redundant with the intercept
- The decision to exclude $C_0(X)$ instead of some other $C_k(X)$ is arbitrary
- Alternatively, we could include $C_0(X), C_1(X), \ldots, C_K(X)$ and exclude the intercept.

Example



The relationship between percentage body fat and body mass index: $N = 326$, number of cut points 50

Step Functions

- Unless there are natural breakpoints in the predictors, piecewise-constant functions can miss the action
- Nevertheless, very popular in biostatistics, epidemiology ...

Basis Functions

- Polynomial and piecewise-constant regression models are special cases of a *basis function approach*
- We have at hand a family of functions or transformations that can be applied to a variable $X : b_1(X), b_2(X), \ldots, b_K(X)$
- We fit the model:

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \cdots + \beta_K b_K(x_i) + \epsilon_i$$

Basis Functions

- The basis functions $b_1(), b_2(), \ldots, b_K()$ are fixed and known
- For polynomial regression: $b_j(x_i) = x_i^j$
- For piecewise constant functions: $b_j(x_i) = I(c_j \leq x_i < c_{(j+1)})$
- A standard linear model with predictors $b_1(x_i), b_2(x_i), ..., b_K(x_i)$:
  - we can use, e.g., least squares to estimate the unknown regression coefficients
  - all the tools for linear models (e.g., standard errors and F-statistics for the model's overall significance) are available in this setting
- Other choices for basis functions: wavelets, Fourier series or **regression splines**

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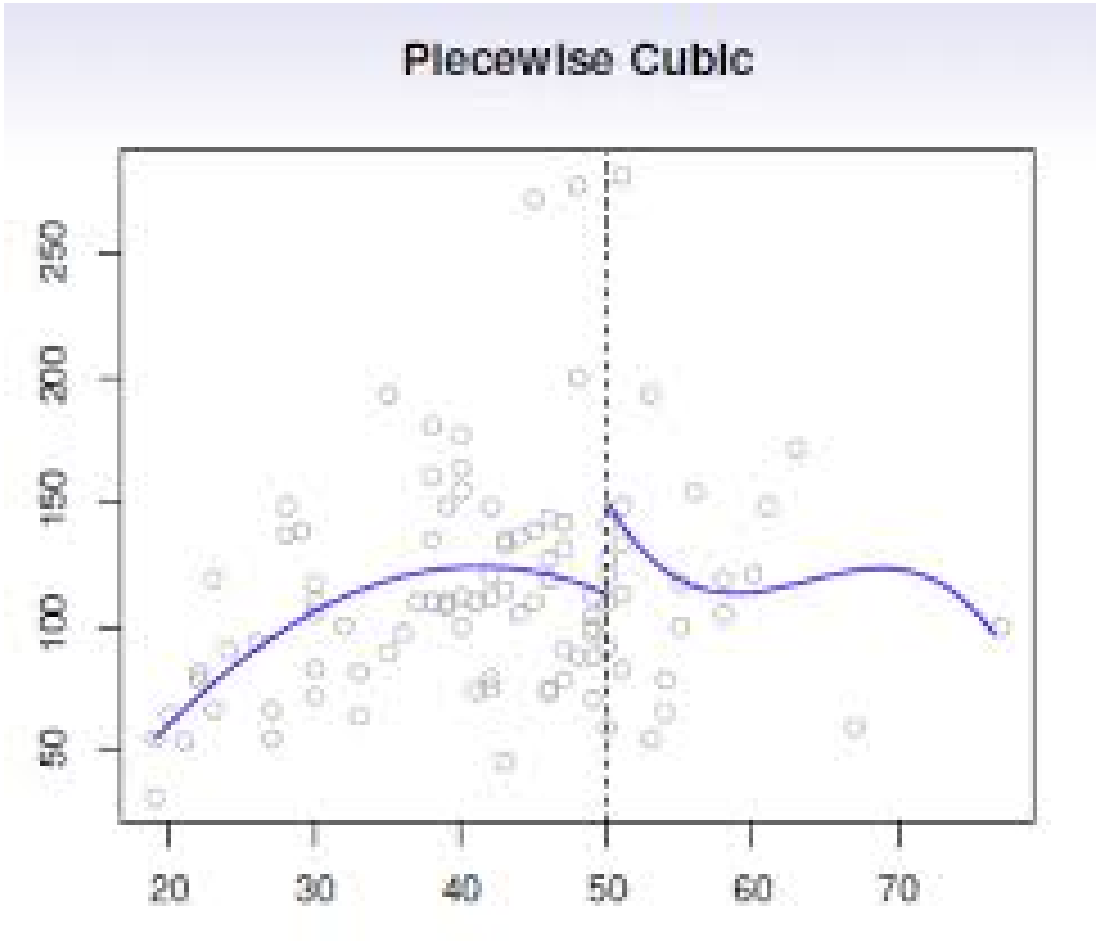
Piecewise Polynomials

- Piecewise polynomial regression involves fitting separate low-degree polynomials over different regions of X
- The points where the coefficients change are called *knots*
- Example, a piecewise cubic polynomial with a single knot at a point c:

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

  - we fit two different polynomial functions to the data:
    - one on the subset of the observations with $x_i < c$
    - one on the subset of the observations with $x_i \geq c$
- Using more knots leads to a more flexible piecewise polynomial

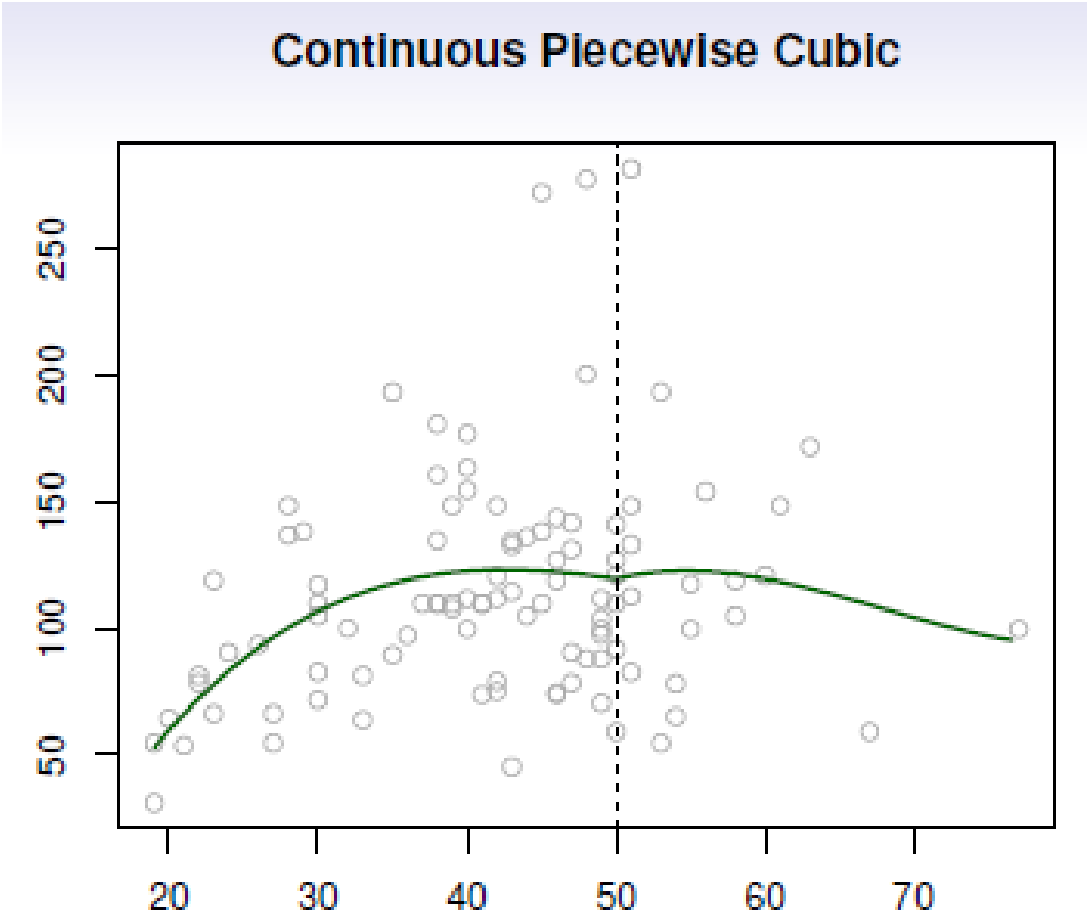
Piecewise Polynomials: example



The function is discontinuous

Constraints and Splines

- Fit a piecewise polynomial under the constraint that the fitted curve must be continuous:

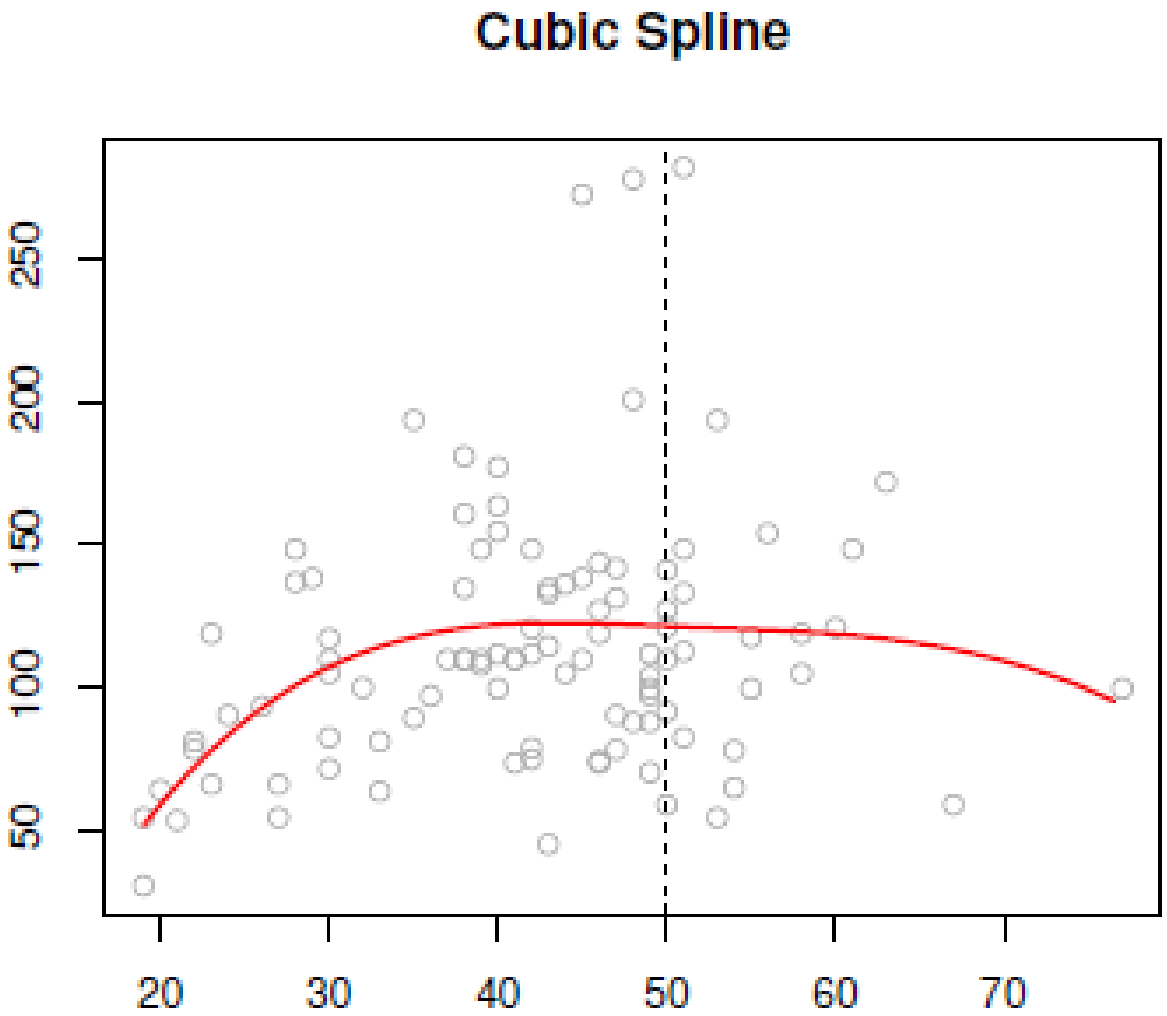


Better, but the V-shaped join looks unnatural

Constraints and Splines

- Additional constraints: both the first and second derivatives of the piecewise polynomials are continuous
- We are requiring that the piecewise polynomial be not only continuous, but also very smooth $\Longrightarrow$ a smoother form of the curve in the join points

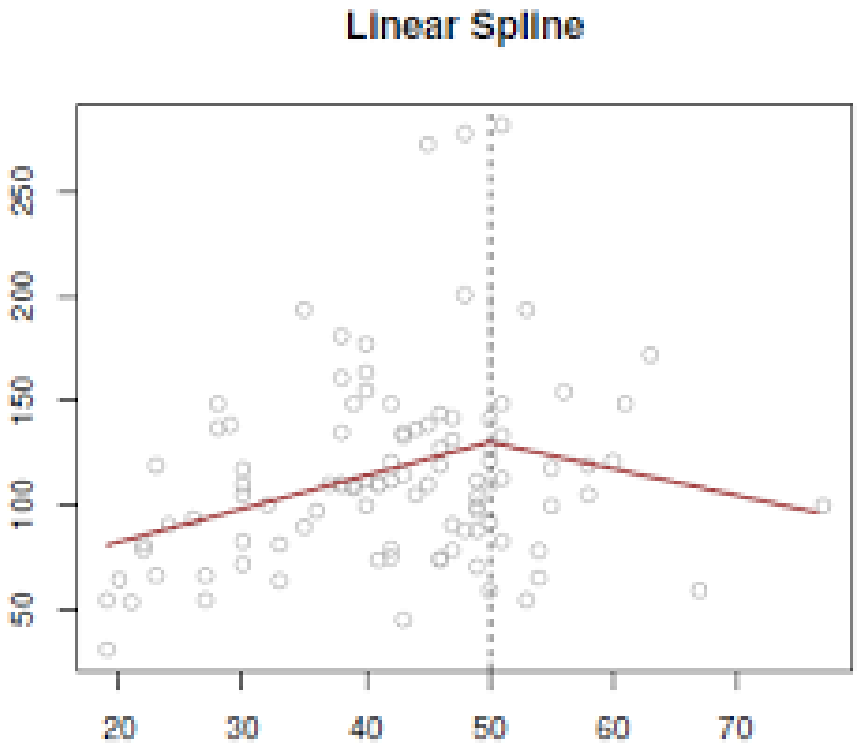
Splines



Splines

A degree-d spline is a piecewise degree-d polynomial, with continuity in derivatives up to degree $d-1$ at each knot

- Example: a linear spline is obtained by fitting a line in each region of the predictor space defined by the knots, requiring continuity at each knot



The Spline Basis Representation

- We can use the basis model to represent a regression spline
- E .g., a cubic spline with K knots can be modeled as

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

for an appropriate choice of basis functions $b_1, b_2, ..., b_{(K+3)}$

- This model can then be fitted using least squares

The Spline Basis Representation

- There are many equivalent ways to represent cubic splines using different choices of basis functions
- The most direct way:
  - start with a basis for a cubic polynomial: x, x^2, x^3
  - add one truncated power basis function per knot:
    - a truncated power basis function:

$$\eta(x,\xi) = (x-\xi)_+^3 = \begin{cases} (x-\xi)^3 & \text{if } x > \xi \\ 0 & \text{otherwise} \end{cases}$$

where ξ is a knot

- There is rarely any need to go beyond cubic splines, which are the most common type of splines in practice.

The Spline Basis Representation

- To fit a cubic spline to a data set with K knots, we perform least squares regression with an intercept and $3 + K$ predictors, of the form

$$X, X^2, X^3, h(X, \xi_1), h(X, \xi_2), ..., h(X, \xi_K)$$

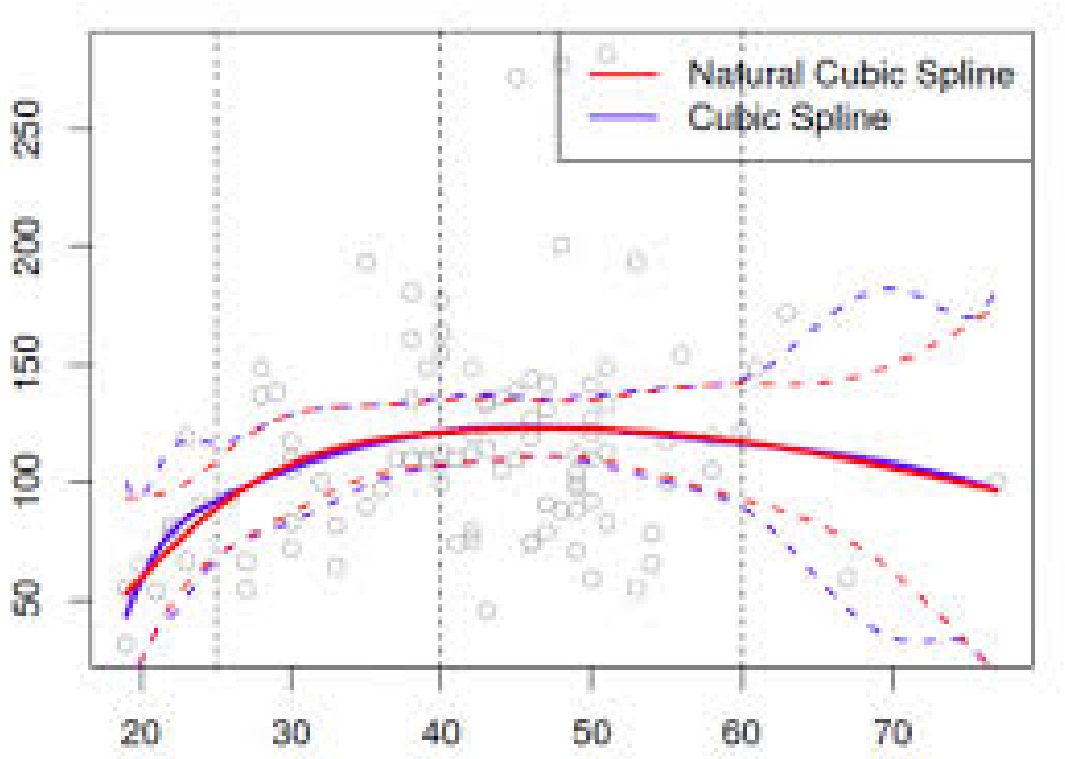
  where $\xi_1, ..., \xi_K$ are the knots

- This amounts to estimating a total of $K + 4$ regression coefficients
- Fitting a cubic spline with K knots uses $K + 4$ degrees of freedom.

Natural Spline

- Splines can have high variance close to the boundary
  - Boundary: the region where X is smaller than the smallest knot, or larger than the largest knot
- *A natural spline* is a regression spline with additional boundary constraints:
  - the function is required to be linear near the boundary
- Natural splines generally produce more stable estimates near the boundaries

Natural Spline



- In blue, a cubic spline: confidence bands in the boundary region appear fairly wild
- In red, a natural cubic spline: the corresponding confidence intervals are narrower

Choosing the Locations of the Knots

- Where should we place the knots?
- The regression spline is most flexible in regions that contain a lot of knots
  - the polynomial coefficients can change rapidly
- One option: to place more knots in places where the function might vary most rapidly, and to place fewer knots where it seems more stable
- In practice, it is common to place knots in a uniform fashion:
  - we specify the desired degrees of freedom
  - the software automatically place the corresponding number of knots at uniform quantiles of the data

Choosing the Number of the Knots

- How many knots should we use (equivalently how many degrees of freedom)?
- One option: try out different numbers of knots and see which produces the best looking curve

Choosing the Number of the Knots

- More objective approach: to use cross-validation:
  - we remove a portion of the data (say 10 %)
  - fit a spline with a certain number of knots to the remaining data
  - use the spline to make predictions for the held-out portion
  - repeat this process multiple times until each observation has been left out once
  - compute the overall cross-validated RSS
  - this procedure can be repeated for different numbers of knots K
  - the value of K giving the smallest RSS is chosen.

Comparison to Polynomial Regression

- Regression splines often give superior results to polynomial regression:
  - polynomials must use a high degree to produce flexible fits
  - splines introduce flexibility by increasing the number of knots but keeping the degree fixed
  - generally, this approach produces more stable estimates
- Splines allow to place more knots, and hence flexibility, over regions where the function f seems to be changing rapidly, and fewer knots where f appears more stable.

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Smoothing Splines

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Smoothing Splines

- Regression splines:
  - specifying a set of knots
  - producing a sequence of basis functions
  - using least squares to estimate the spline coefficients
- A different approach that also produces a spline:

Smoothing Splines

Smoothing Splines

- Fitting a smooth curve to a set of data:
  - we want to find some function, g, that fits the observed data well $\Longleftrightarrow$
  - find function g such that

$$RSS = \sum (y_i - g(x_i))^2 \quad \text{is small}$$

- If we don't put any constraints on g, we can always make RSS zero:
  - by choosing g such that it interpolates all of the y_i
- Such function would overfit the data - it would be far too flexible
- **A function g that makes RSS small, but that is also smooth**

Smoothing Splines

- Find the function g that minimizes

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

  where λ is a nonnegative tuning parameter

- The function g that minimizes this criteria is known as *a smoothing spline*
- It takes the "Loss+Penalty" formulation (as the ridge regression and the lasso)
- The term $\sum_{i=1}^{n} (y_i - g(x_i))^2$ is a loss function that encourages g to fit the data well
- The term $\lambda \int (g''(t))^2 \, \mathrm{d}t$ is a penalty term that penalizes the variability in g.

Smoothing Splines: penalty

$$\lambda \int (g''(t))^2 \, \mathrm{d}t$$

- $g''(t)$ is the second derivative of the function g
- The first derivative $g'(t)$ measures the slope of a function at t
- The second derivative corresponds to the speed at which the slope is changing
- It is a measure of its roughness:
  - it is large in absolute value if g is very wiggly near t
  - it is close to zero otherwise
  - the second derivative of a straight line is zero

Smoothing Splines: penalty

$$\lambda \int (g''(t))^2 \, \mathrm{d}t$$

- Integral: a summation over the range of t
- The penalty is a measure of the total change in the function $g''(t)$ over its entire range
  - if g is close to an affine fit, then $g'(t)$ will be close to constant and $g''(t)^2$ will take a small value
  - if g is jumpy and variable than $g''(t)$ will vary significantly and the $\int$ will take a large value
- **The penalty encourages g to be smooth**
- The larger is the value of λ, the closer g will be to an affine fit (straight line)

Smoothing Splines: penalty

- When $\lambda = 0$ the penalty term has no effect $\implies$ g will be very jumpy and will exactly interpolate the training observations
- When $\lambda \to \infty$, g will be perfectly affine: a straight line that passes as closely as possible to the training points
  - g will be the linear least squares line, since the loss function=RSS
- For an intermediate value of λ, g will approximate the training observations but will be somewhat smooth
- **λ controls the bias - variance trade - off of the smoothing spline**

Smoothing Splines

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

- The function $g(x)$ that minimizes this criteria has special properties:
  1. it is a piecewise cubic polynomial with knots at $x_1, \ldots, x_n$
  2. it has continuous first and second derivatives at each knot
  3. it is linear in the region outside of the extreme knots
- (1) - (3) $\Longrightarrow$ **the function $g(x)$ is a natural cubic spline with knots at $x_1, ..., x_n$!**

Smoothing Splines

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

- It is not the same natural cubic spline that we would get applying the basis function approach with knots at $x_1, ..., x_n$
- A shrunken version, where the value of the tuning parameter λ controls the level of shrinkage.

Choosing the Smoothing Parameter λ

- A smoothing spline: a natural cubic spline with knots at every unique value of x_i
- It might seem that a smoothing spline will have far too many degrees of freedom: a knot at each data point allows a large flexibility
- The tuning parameter λ controls the roughness of the smoothing spline
- We do not need to select the number or the locations of the knots but we need to choose the value of λ

Choosing the Smoothing Parameter λ

- Using cross-validation:
  - find the value of λ that makes the cross-validated RSS as small as possible
- The leave-one-out cross-validation error can be computed very efficiently for smoothing splines with essentially the same cost as computing a single fit

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Local Regression

Local regression is an approach for fitting flexible non-linear functions, which involves computing the fit at a target point x_0 *using only nearby training observations*

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Local Regression

Algorithm: Local Regression at $X = x_0$

1. Gather the fraction $s = k/n$ of training points whose x_i are closest to x_0
2. Assign a weight $K_{(i0)} = K(x_i, x_0)$ to each point in this neighborhood. All but k nearest neighbors get weight zero.
3. Fit a weighted least squares regression of the y_i on the x_i using the weights:

$$\sum_{i=1}^{n} K_{(i0)}(y_i - \beta_0 - \beta_1 x_i)^2$$

4. The fitted value at x_0 is given by $\hat{f}(x_0) = \hat{\beta}_0 + \hat{\beta}_1 x_0$

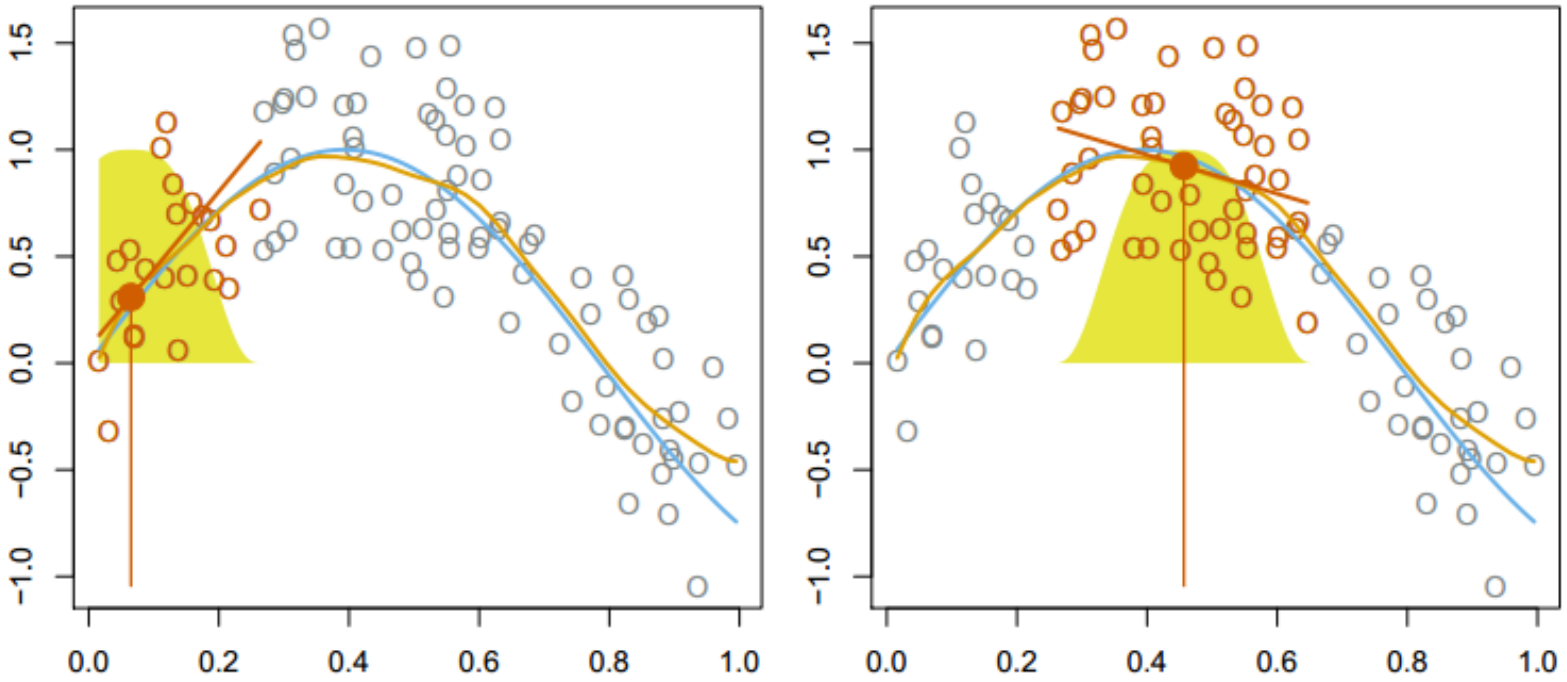
Local Regression

- In Step 3 of Algorithm the weights $K_{(i0)}$ will differ for each value of x_0
- The weight function gives the most weight to the data points nearest the point of estimation and the least weight to the data points that are furthest away:
  - e.g., the tri-cube weight function:

$$w(x) = (1 - |d|^3)^3$$

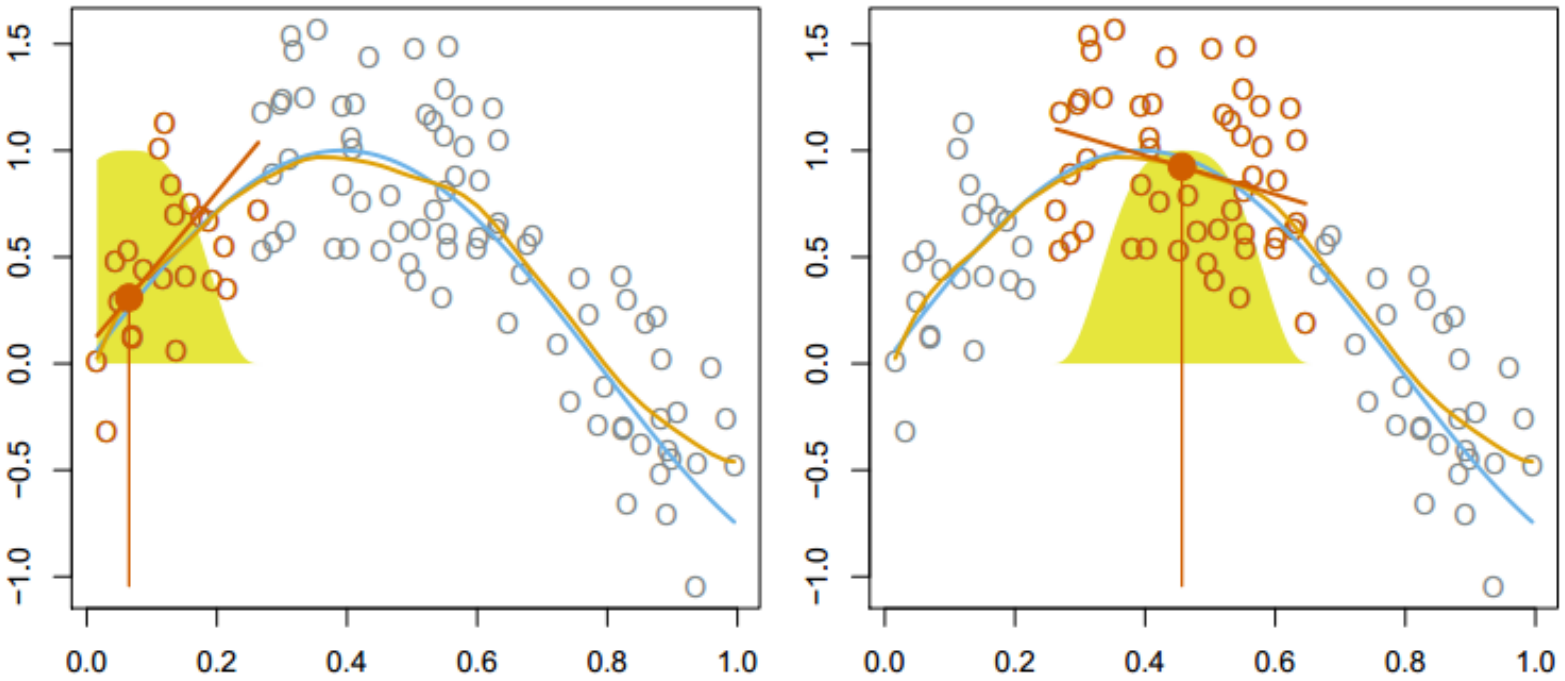
    where d is the distance of a given data point to the point on the curve being fitted, scaled to lie in $[0, 1]$
- Local regression is referred to as a *memory-based procedure*: we need all the training data each time we wish to compute a prediction.

Local Regression: example



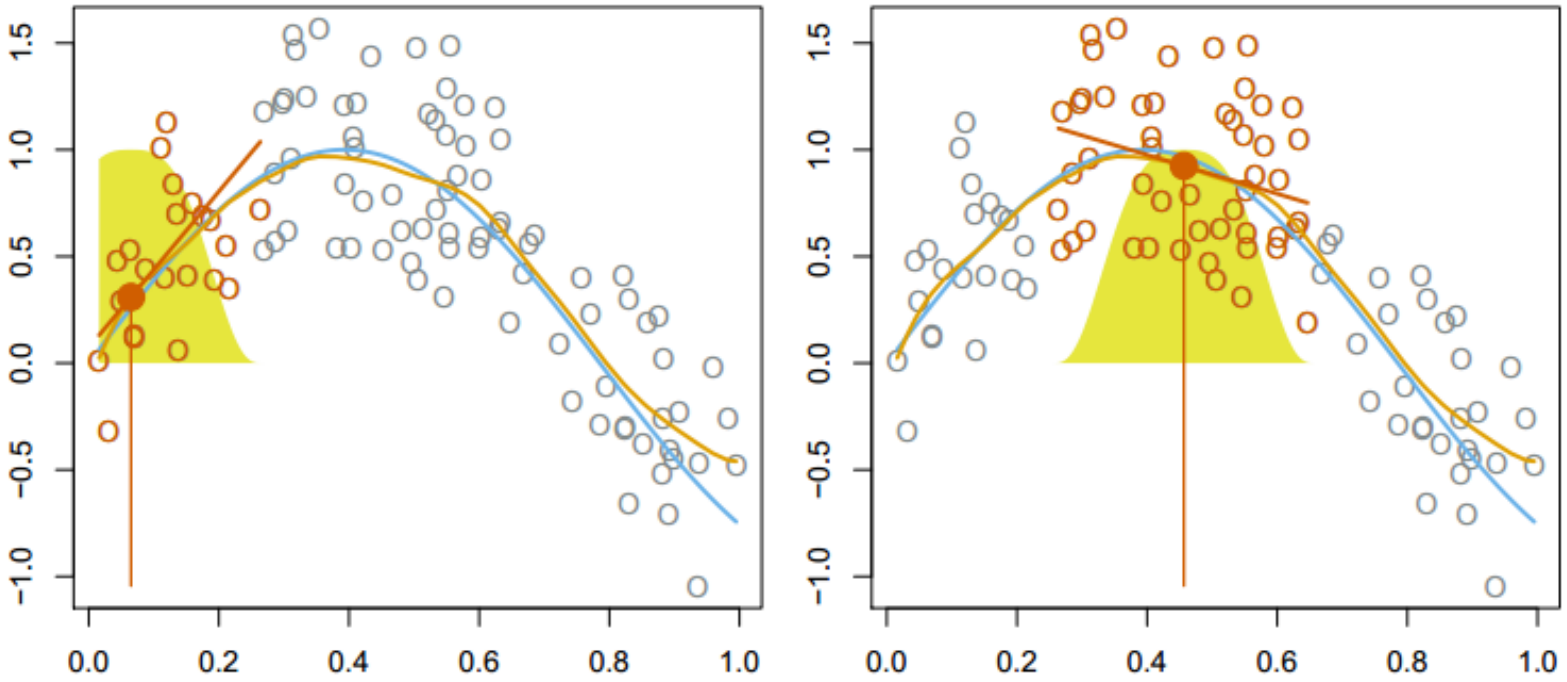
- one target point near 0.4, and another near the boundary at 0.05
- the blue line represents the function $f(x)$ from which the data were generated
- the orange line corresponds to the local regression estimate $\hat{f}(x)$

Local Regression: example



- the orange points are local to the target point x_0
- the green bell-shape indicates weights assigned to each point, decreasing to zero with distance from the target point

Local Regression: example



- the fit at x_0 is obtained by fitting a weighted linear regression (orange line segment)
- the fitted value at x_0 (orange solid dot) is the estimate $\hat{f}(x_0)$

Local Regression

- In order to perform local regression, there are a number of choices to be made:
  - how to define the weighting function K
  - whether to fit a linear, constant, or quadratic regression in Step 3
- The most important choice is the fraction s (Step 1)
  - it plays a role of the tuning parameter λ in smoothing splines: it controls the flexibility of the fit
  - the smaller the value of s, the more local and wiggly will be our fit
  - a very large value of s will lead to a global fit to the data using all of the training observations
  - we can use cross-validation to choose s, or we can specify it directly.

Local Regression: generalizations

Multiple features $X_1, X_2, ..., X_p$:

- fitting a multiple linear regression model that is global in some variables, but local in another, such as time:

Varying coefficient models

- allows to adapt the model to the most recently gathered data

Local Regression: generalizations

Models that are local in a pair of variables X_1 and X_2 rather than one:

- use two-dimensional neighborhoods to fit bivariate linear regression models using the observations that are near each target point in two-dimensional space
- the same approach can be implemented in higher dimensions, using linear regressions fit to p-dimensional neighborhoods
  - local regression can perform poorly if p is large as there will generally be very few training observations close to x_0 (similar to Nearest-neighbors regression)

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Generalized Additive Models

- Flexibly predicting a response Y on the basis of a single predictor X: extensions of simple linear regression
- Flexibly predicting Y on the basis of several predictors $X_1, ..., X_p$:

Generalized additive models (GAMs)

- an extension of multiple linear regression
- a general framework for extending a standard linear model by allowing non-linear functions of each of the variables, while maintaining additivity
- GAMs can be applied with both quantitative and qualitative responses.

Generalized additive models

Replace each linear component $\beta_j X_j$ with a (smooth) non-linear function $f_j(X_j)$:

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

- It is an additive model because we calculate a separate f_j for each X_j and then add together all of their contributions
- Methods for fitting functions to a single variable can be used as building blocks for fitting an additive model.

Example: Wage data

Predicting wage as function of year, age and education:

$$\text{wage} = \beta_0 + f_1(\text{year}) + f_2(\text{age}) + f_3(\text{education}) + \epsilon$$

- year and age are quantitative variables
- education is the level of high school or college education that an individual has completed:
  - a qualitative variable with five levels: $<$HS, HS,$<$Coll, Coll, $>$Coll
- We fit f_1 and f_2 using natural splines
- We fit f_3 using a separate constant for each level, via the usual dummy variable approach

Example: Wage data

Predicting wage as function of years in working force, age and education:

$$\text{wage} = \beta_0 + f_1(\text{year}) + f_2(\text{age}) + f_3(\text{education}) + \epsilon$$

- We can use least squares:
  - natural splines can be constructed using an appropriately chosen set of basis functions
  - the entire model is just a big regression onto spline basis variables and dummy variables

Example: Wage data

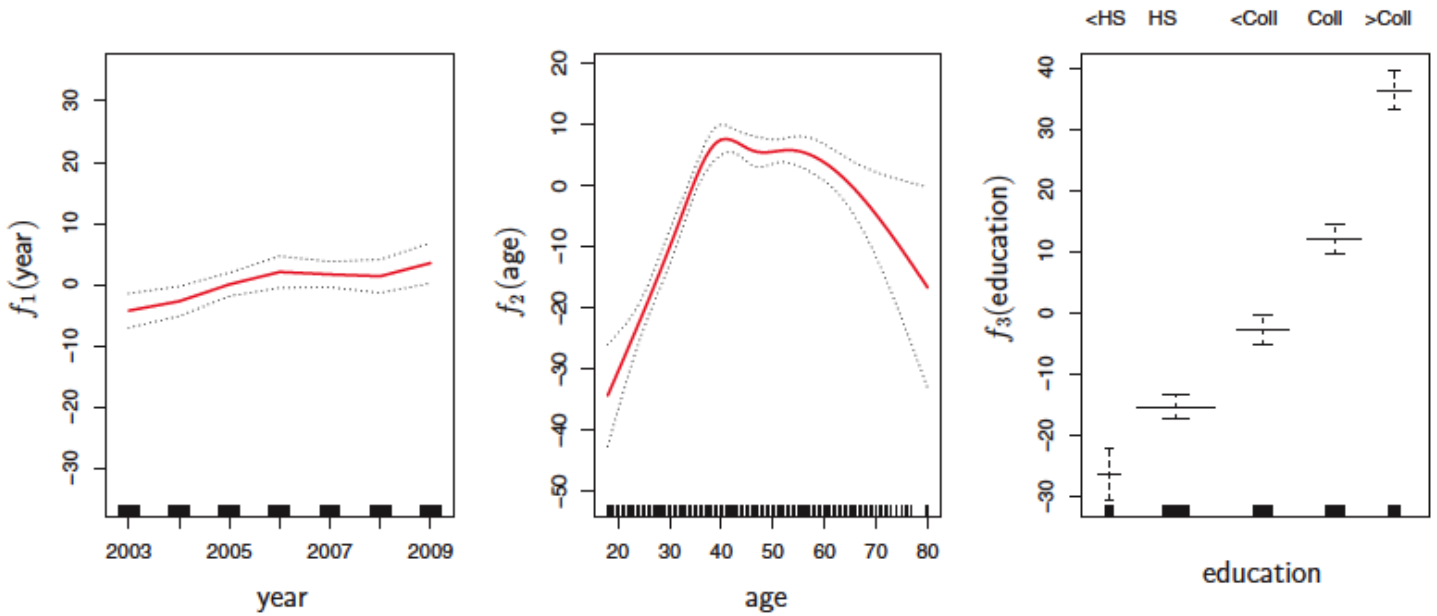
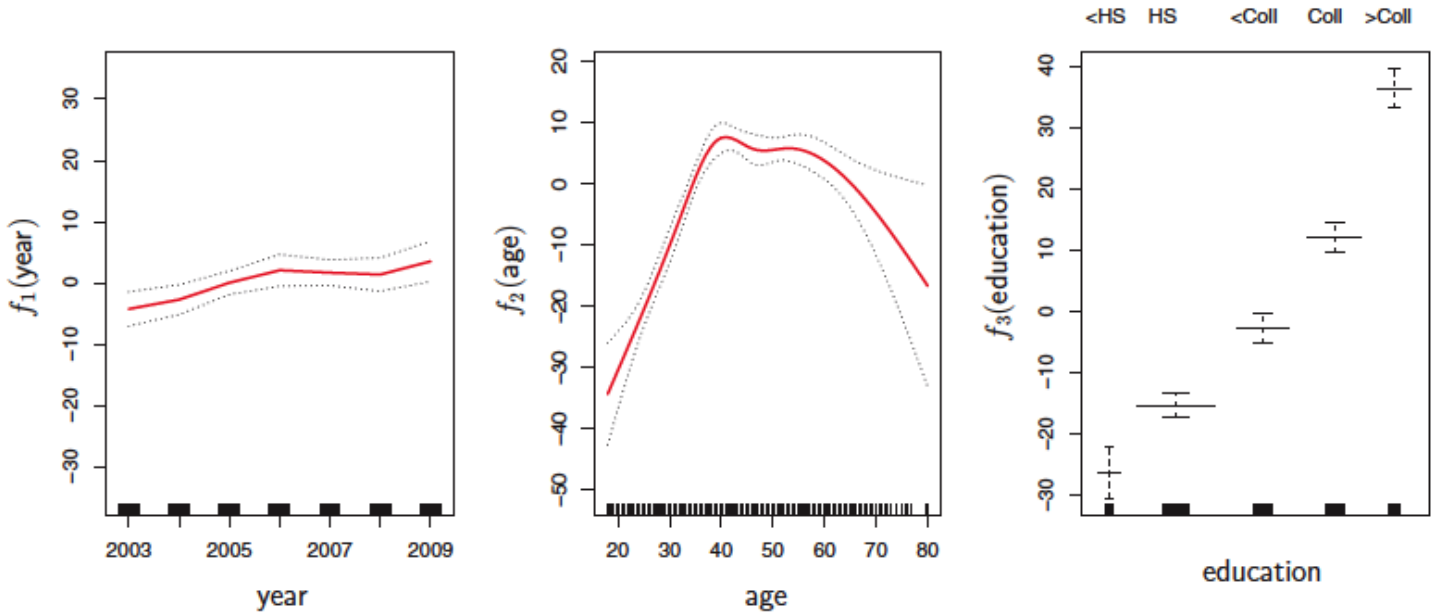


FIGURE 7.11. *For the* `Wage` *data, plots of the relationship between each feature and the response,* `wage`*, in the fitted model (7.16). Each plot displays the fitted function and pointwise standard errors. The first two functions are natural splines in* `year` *and* `age`*, with four and five degrees of freedom, respectively. The third function is a step function, fit to the qualitative variable* `education`*.*

- The left-hand panel: holding age and education fixed, wage tends to increase slightly with year

Example: Wage data



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- The center panel: holding education and year fixed, wage tends to be highest for intermediate values of age, and lowest for the very young and very old.

Example: Wage data

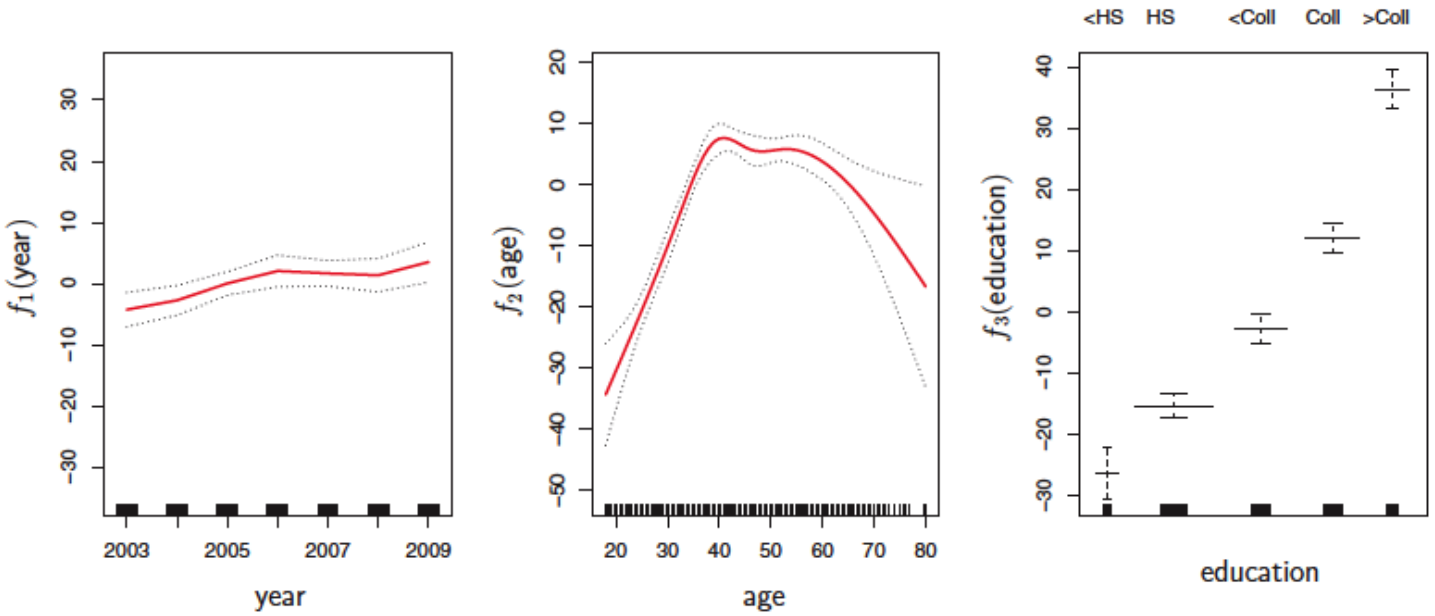

FIGURE 7.11. *For the* `Wage` *data, plots of the relationship between each feature and the response,* `wage`*, in the fitted model (7.16). Each plot displays the fitted function and pointwise standard errors. The first two functions are natural splines in* `year` *and* `age`*, with four and five degrees of freedom, respectively. The third function is a step function, fit to the qualitative variable* `education`*.*

- The right-hand panel: holding year and age fixed, wage tends to increase with education

GAMs

- As the building blocks for GAMs we can use local regression, polynomial regression, or any combination of these approaches
- Advantages:
  - GAMs allow us to fit a non-linear f_j to each X_j
  - We do not need to manually try out many different transformations on each variable individually
  - The non-linear fits can potentially give more accurate predictions for the response Y
  - As 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
  - If we are interested in inference, GAMs provide a useful representation

Limitation of GAMs

- The model is restricted to be additive
- With many variables, important interactions can be missed
- We can manually add interaction terms to the GAM model by including additional predictors of the form $X_j \times X_k$
- We can add low-dimensional interaction functions of the form $f_{(jk)}(X_j, X_k)$ into the model
  - can be fitted using two-dimensional local regression, or two-dimensional splines
- For fully general models, we have to look for even more flexible approaches such as random forests and boosting.

References

- Trevor Hastie, Robert Tibshirani, Jerome Friedman. *The elements of statistical learning - Data Mining, inference, and prediction.* Springer.

- Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. *An Introduction to Statistical Learning with applications in R.* Springer.