Chapter 7 – Moving beyond linearity

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Outline

1. 7.1 – Polynomial regression
2. 7.2 – Step functions
3. 7.3 – Basis functions
4. 7.4 – Splines
5. 7.5 – Smoothing splines
6. Multidimensional splines

Polynomial regression

Linear function: $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$

Polynomial function:

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

Logistic regression using polynomials:

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

Example

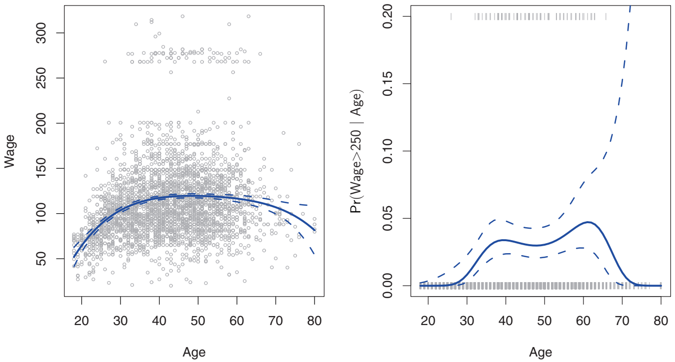

FIGURE 7.1. *The* `Wage` *data.* Left: *The solid blue curve is a degree-4 polynomial of* `wage` *(in thousands of dollars) as a function of* `age`*, fit by least squares. The dotted curves indicate an estimated 95 % confidence interval.* Right: *We model the binary event* `wage>250` *using logistic regression, again with a degree-4 polynomial. The fitted posterior probability of* `wage` *exceeding* $250,000 *is shown in blue, along with an estimated 95 % confidence interval.*

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Regression using indicator functions

Indicator functions:

$$
\begin{aligned}
C_0(X) &= I(X < c_1), \\
C_1(X) &= I(c_1 \leq X < c_2), \\
C_2(X) &= I(c_2 \leq X < c_3), \\
&\vdots \\
C_{K-1}(X) &= I(c_{K-1} \leq X < c_K), \\
C_K(X) &= I(c_K \leq X),
\end{aligned}
$$

Regression:

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

Logistic regression:

$$\Pr(y_i > 250 | x_i) = \frac{\exp(\beta_0 + \beta_1 C_1(x_i) + \ldots + \beta_K C_K(x_i))}{1 + \exp(\beta_0 + \beta_1 C_1(x_i) + \ldots + \beta_K C_K(x_i))}$$

Example

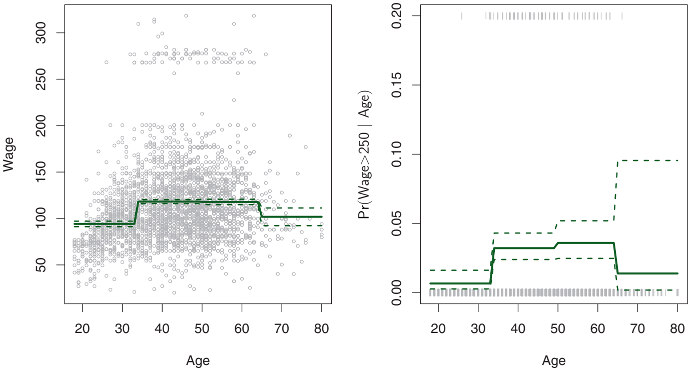

FIGURE 7.2. *The* `Wage` *data.* Left: *The solid curve displays the fitted value from a least squares regression of* `wage` *(in thousands of dollars) using step functions of* `age`*. The dotted curves indicate an estimated 95 % confidence interval.* Right: *We model the binary event* `wage>250` *using logistic regression, again using step functions of* `age`*. The fitted posterior probability of* `wage` *exceeding* \$250,000 *is shown, along with an estimated 95 % confidence interval.*

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Regression using basis functions

Basis functions: $b_1(\cdot), \ldots, b_K(\cdot)$

Regression using basis functions:

$$y_i = \beta_0 + \beta_1 b_1(x_i) + \beta_2 b_2(x_i) + \beta_3 b_3(x_i) + \ldots + \beta_K b_K(x_i) + \epsilon_i.$$

Popular basis:

- Polynomials
- Fourier basis
- Wavelet basis
- Splines

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7.4.1 – Piecewise polynomials

Cubic polynomial:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \epsilon_i,$$

Piecewise polynomial with a single knot at c:

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

Constraints:

- $\hat{f}$ is continuous
- $\hat{f}'$, $\hat{f}''$, ... are continuous

Example

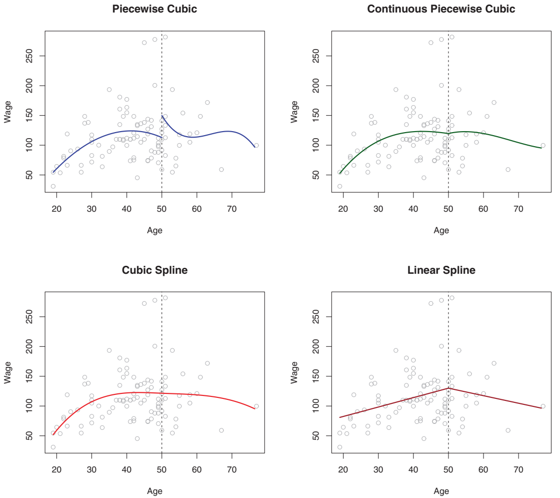

FIGURE 7.3. *Various piecewise polynomials are fit to a subset of the* `Wage` *data, with a knot at* `age=50`. Top Left: *The cubic polynomials are unconstrained.* Top Right: *The cubic polynomials are constrained to be continuous at* `age=50`. Bottom Left: *The cubic polynomials are constrained to be continuous, and to have continuous first and second derivatives.* Bottom Right: *A linear spline is shown, which is constrained to be continuous.*

Piecewise linear

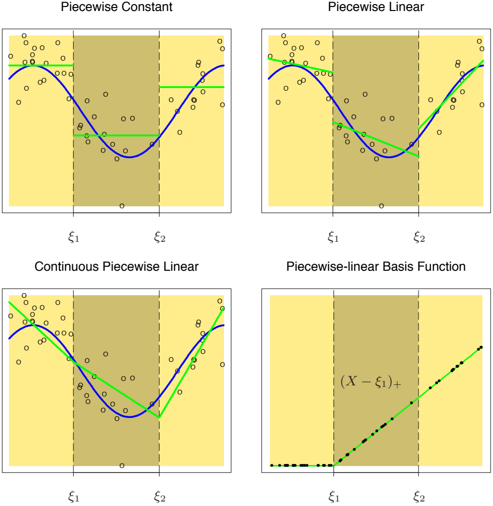

FIGURE 5.1. *The top left panel shows a piecewise constant function fit to some artificial data. The broken vertical lines indicate the positions of the two* knots *ξ_1 and ξ_2. The blue curve represents the true function, from which the data were generated with Gaussian noise. The remaining two panels show piecewise linear functions fit to the same data—the top right unrestricted, and the lower left restricted to be continuous at the knots. The lower right panel shows a piecewise–linear basis function, $h_3(X) = (X - \xi_1)_+$, continuous at ξ_1. The black points indicate the sample evaluations $h_3(x_i)$, $i = 1, \ldots, N$.*

Piecewise cubic polynomials

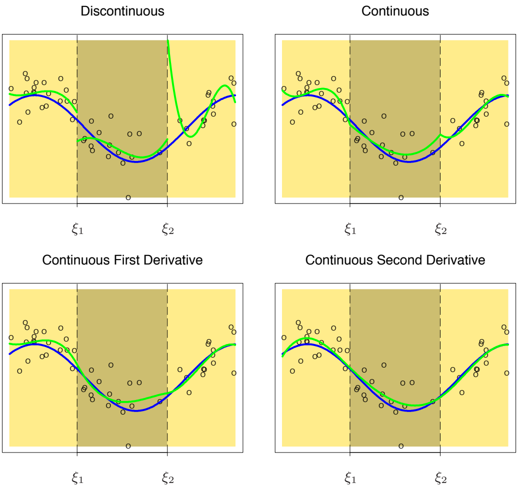

FIGURE 5.2. *A series of piecewise-cubic polynomials, with increasing orders of continuity.*

7.4.1 – The spline basis representation

General model: Fit a piecewise degree d polynomial under the constraint that its first $d-1$ derivatives are continuous

Cubic spline: K knots at $\xi_1, \ldots, \xi_K$

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

Truncated power basis:

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

Basis functions for cubic spline:

$$1, X, X^2, X^3, h(x,\xi_1), h(x,\xi_2), \ldots, h(x,\xi_K)$$

Coefficients: $\beta_0, \ldots, \beta_{K+3}$, degree of freedom $= K+4$

Natural cubic spline

Natural cubic spline: is a regression spline with additional boundary constraints: for example, the function is linear at the boundary

Degree of freedom: K

Example:

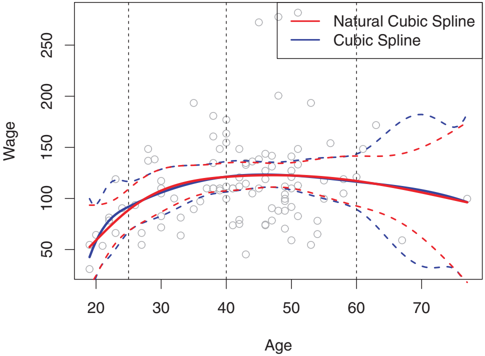

FIGURE 7.4. *A cubic spline and a natural cubic spline, with three knots, fit to a subset of the* `Wage` *data.*

7.4.4 – Choosing the number and locations of the knots

Questions:

- Where should we place the knots? – Adaptive methods
- How many knots should we use, or equivalently how many degrees of freedom should our spline contain? – Cross validation

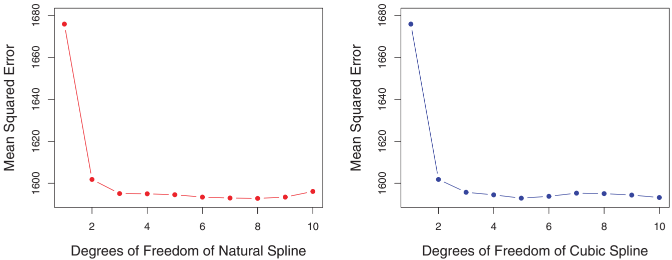

FIGURE 7.6. *Ten-fold cross-validated mean squared errors for selecting the degrees of freedom when fitting splines to the* `Wage` *data. The response is* `wage` *and the predictor* `age`. Left: *A natural cubic spline.* Right: *A cubic spline.*

7.4.5 – Spline and polynomial regression

- Splines are more flexible and stable
- Polynomials may have the Runge phenomenon.

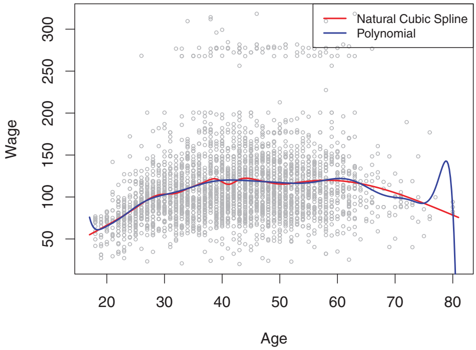

FIGURE 7.7. *On the* `Wage` *data set, a natural cubic spline with 15 degrees of freedom is compared to a degree-15 polynomial. Polynomials can show wild behavior, especially near the tails.*

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Regularization

$$\mathrm{RSS}(f, \lambda) = \sum_{i=1}^{N} \{y_i - f(x_i)\}^2 + \lambda \int \{f''(t)\}^2 dt,$$

λ : a smoothing parameter

- $\lambda = 0$: f can be any function that interpolates the data
- $\lambda = \infty$: will obtain a line such that $f'' = 0$

Solution: See Exercise 5.7 in the book "The elements of statistical learning "

Exercise 5.7 in "The elements of statistical learning "

Ex. 5.7 *Derivation of smoothing splines* (Green and Silverman, 1994). Suppose that $N \geq 2$, and that g is the natural cubic spline interpolant to the pairs $\{x_i, z_i\}_1^N$, with $a < x_1 < \cdots < x_N < b$. This is a natural spline

with a knot at every x_i; being an N-dimensional space of functions, we can determine the coefficients such that it interpolates the sequence z_i exactly. Let $\tilde{g}$ be any other differentiable function on $[a, b]$ that interpolates the N pairs.

(a) Let $h(x) = \tilde{g}(x) - g(x)$. Use integration by parts and the fact that g is a natural cubic spline to show that

$$\begin{aligned} \int_a^b g''(x)h''(x)dx &= -\sum_{j=1}^{N-1} g'''(x_j^+)\{h(x_{j+1}) - h(x_j)\} \quad (5.72) \\ &= 0. \end{aligned}$$

(b) Hence show that

$$\int_a^b \tilde{g}''(t)^2 dt \geq \int_a^b g''(t)^2 dt,$$

and that equality can only hold if h is identically zero in $[a, b]$.

(c) Consider the penalized least squares problem

$$\min_f \left[\sum_{i=1}^N (y_i - f(x_i))^2 + \lambda \int_a^b f''(t)^2 dt \right].$$

Use (b) to argue that the minimizer must be a cubic spline with knots at each of the x_i.

How to find the cubic spline?

Basis expansion:

$$f(x) = \sum_{j=1}^{N} N_j(x)\theta_j,$$

Define matrix: $\{\mathbf{N}\}_{ij} = N_j(x_i)$ and $\{\boldsymbol{\Omega}_\mathbf{N}\}_{jk} = \int N_j''(t)N_k''(t)dt$

$$\mathrm{RSS}(f,\lambda) = \sum_{i=1}^{N}\{y_i - f(x_i)\}^2 + \lambda\int\{f''(t)\}^2dt,$$

is equivalent to

$$\mathrm{RSS}(\theta,\lambda) = (\mathbf{y}-\mathbf{N}\theta)^T(\mathbf{y}-\mathbf{N}\theta) + \lambda\theta^T\boldsymbol{\Omega}_N\theta,$$

Solution:

$$\hat{\theta} = (\mathbf{N}^T\mathbf{N} + \lambda\boldsymbol{\Omega}_N)^{-1}\mathbf{N}^T\mathbf{y},$$

Degree of freedom: = the number of coefficients

Example

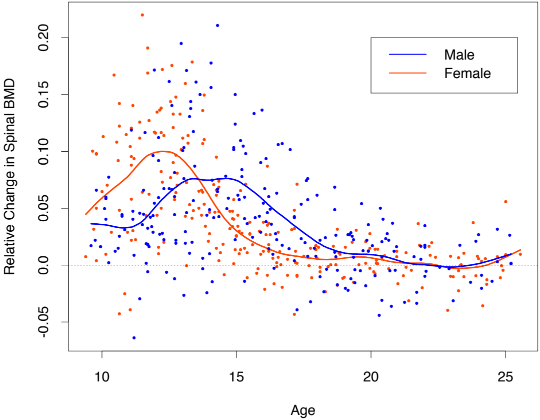


FIGURE 5.6. *The response is the relative change in bone mineral density measured at the spine in adolescents, as a function of age. A separate smoothing spline was fit to the males and females, with* $\lambda \approx 0.00022$*. This choice corresponds to about 12 degrees of freedom.*

7.5.2 – Choosing the smoothing parameter λ

$\hat{\mathbf{f}}$: the N-vector of fitted values $\hat{f}(x_i)$ at the training points $\{x_i\}_{i=1}^{N}$

$$\begin{aligned} \hat{\mathbf{f}} &= \mathbf{N}(\mathbf{N}^T\mathbf{N} + \lambda\mathbf{\Omega}_N)^{-1}\mathbf{N}^T\mathbf{y} \\ &= \mathbf{S}_\lambda \mathbf{y}. \end{aligned}$$

Smoother matrix: $\mathbf{S}_\lambda$

An example of the smoother matrix

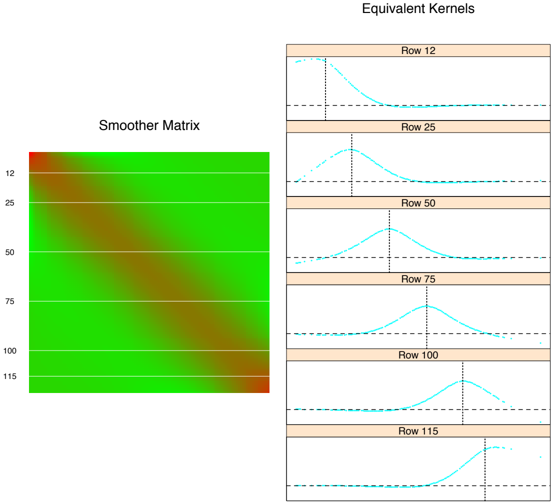


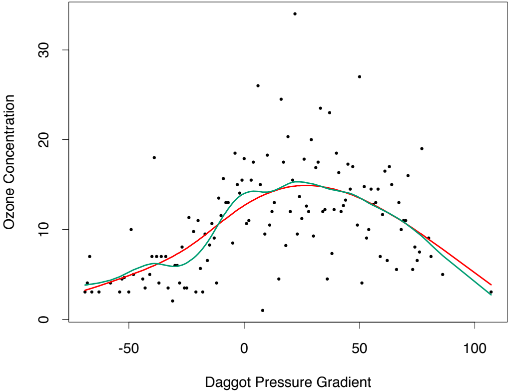
FIGURE 5.8. *The smoother matrix for a smoothing spline is nearly banded, indicating an equivalent kernel with local support. The left panel represents the elements of* **S** *as an image. The right panel shows the equivalent kernel or weighting function in detail for the indicated rows.*

How to choose λ?

Effective degree of freedom: the sum of diagonals of $\mathbf{S}_\lambda$

$$\mathrm{df}_\lambda = \mathrm{trace}(\mathbf{S}_\lambda),$$

Red: $df_\lambda = 5$; Green: $df_\lambda = 11$



How to choose λ? Cross validation.

Example

$$
\begin{aligned}
Y &= f(X) + \varepsilon, \\
f(X) &= \frac{\sin(12(X + 0.2))}{X + 0.2}, \\
X \sim U[0,1] & \text{ and } \varepsilon \sim N(0,1)
\end{aligned}
$$

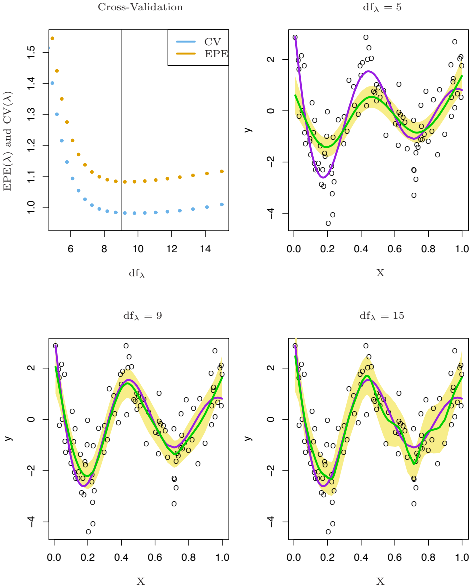


FIGURE 5.9. *The top left panel shows the* EPE(λ) *and* CV(λ) *curves for a realization from a nonlinear additive error model (5.22). The remaining panels show the data, the true functions (in purple), and the fitted curves (in green) with yellow shaded* $\pm 2\times$ *standard error bands, for three different values of* df_λ.

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Tensor product basis

2D splines: $X \in \mathbb{R}^2$

- Basis functions of coordinate X_1: $h_{1,k}(X_1), k = 1, \ldots, M_1$
- Basis functions of coordinate X_2: $h_{2,k}(X_2), k = 1, \ldots, M_2$

Tensor product basis:

$$g_{jk}(X) = h_{1j}(X_1)h_{2k}(X_2),\ j = 1, \ldots, M_1,\ k = 1, \ldots, M_2$$

To represent functions:

$$g(X) = \sum_{j=1}^{M_1} \sum_{k=1}^{M_2} \theta_{jk} g_{jk}(X).$$

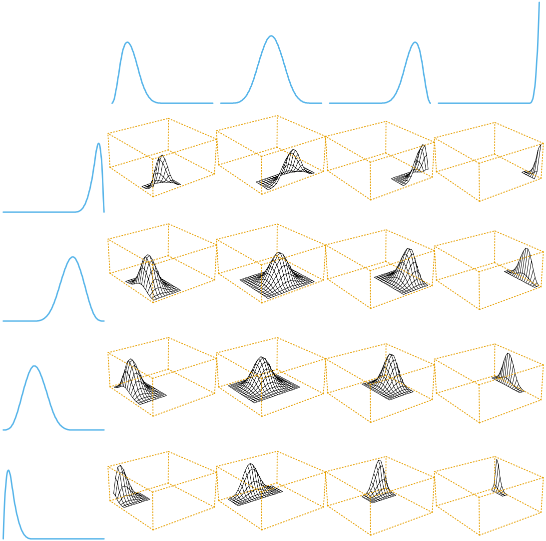

FIGURE 5.10. *A tensor product basis of B-splines, showing some selected pairs. Each two-dimensional function is the tensor product of the corresponding one dimensional marginals.*

Smoothing splines in two dimensions

$$\min_f \sum_{i=1}^{N} \{y_i - f(x_i)\}^2 + \lambda J[f],$$

$$J[f] = \int\int_{\mathbb{R}^2} \left[\left(\frac{\partial^2 f(x)}{\partial x_1^2} \right)^2 + 2 \left(\frac{\partial^2 f(x)}{\partial x_1 \partial x_2} \right)^2 + \left(\frac{\partial^2 f(x)}{\partial x_2^2} \right)^2 \right] dx_1 dx_2.$$

- As $\lambda \to 0$, the solution approaches an interpolating function
- As $\lambda \to \infty$, the solution approaches the least squares plane

Reference

Chapter 7: James, Gareth, Daniela Witten, Trevor Hastie and Robert Tibshirani, An introduction to statistical learning. Vol. 112, New York: Springer, 2013

Chapter 5: Trevor Hastie, Robert Tibshirani, The Elements of Statistical Learning, Second Edition.