

Shape-constrained splines

Applications and examples in R

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Outline

- 1 Splines in regression models
- 2 Defining constraints to the shape
- 3 Shape constrained additive models
- 4 Some examples in R
- 5 Extensions and discussion

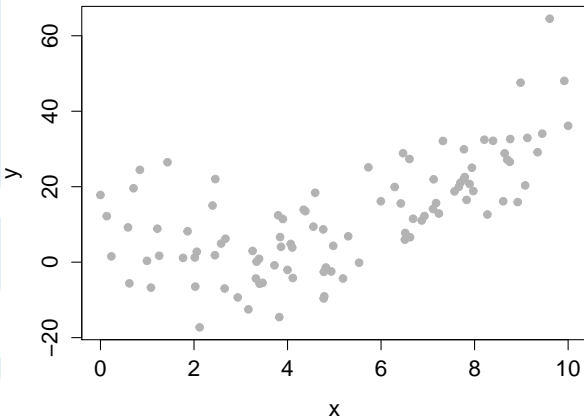


Outline

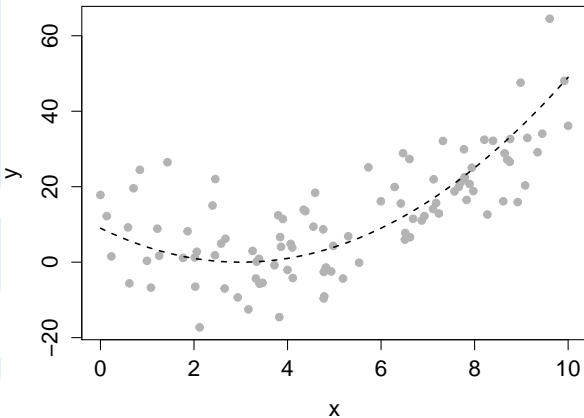
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Scatterplot of x and y



True relationship



B-spline regression

The relationship between the predictor x_i and the response y_i , with $i = 1, \dots, n$, can be defined by a function f :

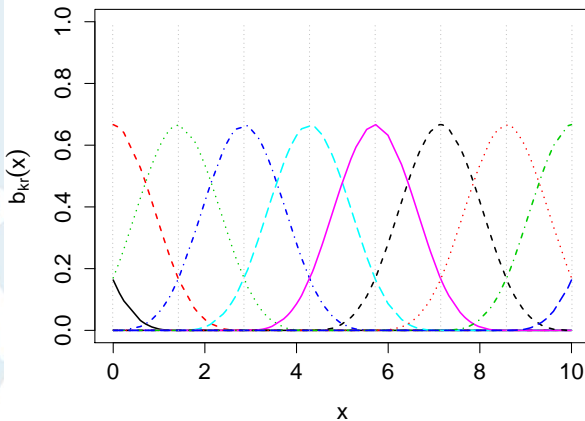
$$y_i = f(x_i)$$

The function can be approximated by $m = p + r$ **B-splines** of degree r , by setting $p + 1$ knots in the range $x_1 \leq x \leq x_n$:

$$y_i = f(x_i) \approx \sum_{k=1}^m \gamma_k b_{k,r}(x_i)$$

where $b_{k,r}$ is the (non-negative) k^{th} B-spline and γ_k its coefficient

Spline basis terms



Estimation

By defining:

$$\boldsymbol{\gamma} = [\gamma_1, \dots, \gamma_k, \dots, \gamma_m]^T$$

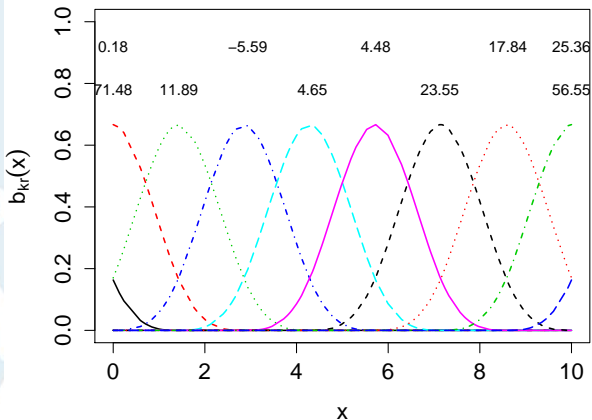
$$\mathbf{x}_i = [b_{1,r}(x_i), \dots, b_{k,r}(x_i), \dots, b_{m,r}(x_i)]^T$$

it is possible to rely on **standard estimation methods** by minimizing the least square objective:

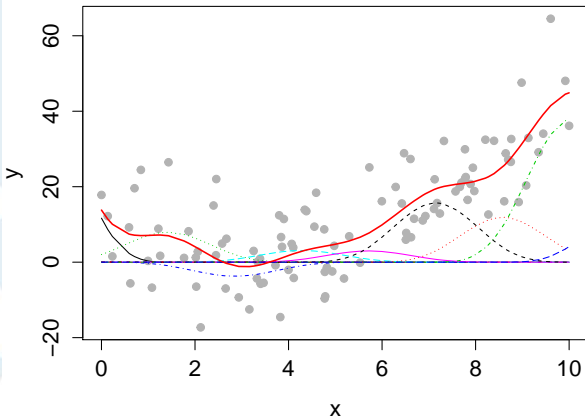
$$\sum_{i=1}^n (y_i - f(x_i; \boldsymbol{\gamma}))^2 = \|\mathbf{y} - \mathbf{X}\boldsymbol{\gamma}\|^2$$



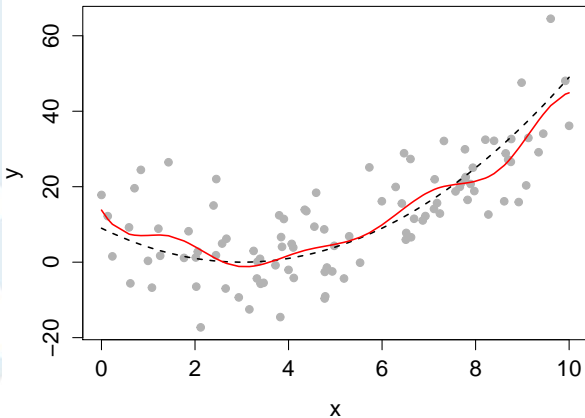
Splines and coefficients



Fitted curve



Comparison



Issues and motivation

Two issues:

- 1 'Wiggly' shape: need to define **optimal smoothness** of the curve [NB: discussed in a previous CSM seminar]
- 2 Possibility of imposing **shape-constraints** on the curve [NB: today's topic]

The latter can be based on a priori assumptions: in many biological or epidemiological phenomena, we can assume for instance **monotonic increasing/decreasing** and/or **convex/concave** associations



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Derivatives of a spline function

For a B-spline function:

$$f(x; \gamma) = \sum_{k=1}^m \gamma_k b_{k,r}(x)$$

assuming equi-spaced knots at distance z , the derivatives can be computed as:

$$f'(x; \gamma) = z^{-1} \sum_{k=2}^m (\gamma_k - \gamma_{k-1}) b_{k,r-1}(x)$$

$$f''(x; \gamma) = z^{-2} \sum_{k=3}^m (\gamma_k - 2\gamma_{k-1} + \gamma_{k-2}) b_{k,r-2}(x)$$



Imposing constraints

Constraints on the first derivative

A sufficient condition for $f'(x; \gamma) > 0$ is $\gamma_k - \gamma_{k-1} > 0$ for $k = 2, \dots, m$

Constraints on the second derivative

A sufficient condition for $f''(x; \gamma) > 0$ is $\gamma_k - 2\gamma_{k-1} + \gamma_{k-2} > 0$ for $k = 3, \dots, m$

Constraints on **linear combinations of the coefficients** map into constraints on the **shape of the relationship**

In matrix terms

Defining the two difference matrices:

$$\mathbf{D}_1 = \begin{pmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{pmatrix}; \quad \mathbf{D}_2 = \begin{pmatrix} 1 & -2 & 1 & \cdots & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 \end{pmatrix}.$$

Then:

$$f'(x; \gamma) > 0 \quad \Rightarrow \quad \mathbf{D}_1 \gamma > \mathbf{0}$$

$$f''(x; \gamma) > 0 \quad \Rightarrow \quad \mathbf{D}_2 \gamma > \mathbf{0}$$



Type of constraints

- Monotonically increasing: $f'(x_i; \gamma) > 0 \Rightarrow \mathbf{D}_1 \gamma > \mathbf{0}$
- Monotonically decreasing: $f'(x_i; \gamma) < 0 \Rightarrow -\mathbf{D}_1 \gamma > \mathbf{0}$
- Convex: $f''(x_i; \gamma) > 0 \Rightarrow \mathbf{D}_2 \gamma > \mathbf{0}$
- Concave: $f''(x_i; \gamma) < 0 \Rightarrow -\mathbf{D}_2 \gamma > \mathbf{0}$
- Monotonically increasing and convex: $f'(x_i; \gamma) > 0$ and $f''(x_i; \gamma) > 0 \Rightarrow [\mathbf{D}_1^T \mathbf{D}_2^T]^T \gamma > \mathbf{0}$
- ...

Estimation can be performed through **linear constrained optimization** using the log-likelihood function



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An extension by Pya and Wood

Pya and Wood (2010, 2015) proposed **shape constrained additive models**

This approach simultaneously addresses two issues:

- 1 imposing constraints on the shape through a **re-parameterization** of the model
- 2 defining the optimal smoothness of the curve via additive models with **penalized splines**



Re-parameterization as an unconstrained model

In the case of monotonically increasing shapes, the constraints are enforced by setting $\gamma_k - \gamma_{k-1} > 0$ for $k = 2, \dots, m$

This can also be obtained by re-parameterizing the B-splines with **unconstrained coefficients** ϕ as:

$$\gamma_1 = \phi_1, \gamma_k = \phi_1 + \sum_{j=2}^k e^{\phi_j}, k = 2, \dots, m$$

Matrix formulation

Setting $\gamma = \mathbf{P}\tilde{\phi}$, with $\tilde{\phi} = [\phi_1, e^{\phi_2}, \dots, e^{\phi_m}]^T$, and:

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \dots & 1 \end{pmatrix}$$

the regression model can be written in terms of unconstrained *working* parameters as:

$$f(x; \phi) = \mathbf{X}\mathbf{P}\tilde{\phi}$$

Fitted through **non-linear unconstrained optimization**

Shape constrained penalized splines

The **optimal smoothness** of the relationship can be found by penalizing differences between adjacent coefficients (Wood 2006)

The least square objective can be modified to:

$$\|\mathbf{y} - \mathbf{X}\mathbf{P}\tilde{\boldsymbol{\phi}}\|^2 + \lambda\boldsymbol{\phi}^T\mathbf{S}\boldsymbol{\phi}$$

where $\mathbf{S} = \mathbf{D}_2^T\mathbf{D}_2$ is a known **penalty matrix** (with \mathbf{D}_2 previously defined), and λ is a **smoothing parameter**



Maximizing the log-likelihood

$$\mathcal{L}_p(\phi, \lambda) = \mathcal{L}(\phi) - \frac{1}{2} \lambda \phi^T \mathbf{S} \phi$$

$$J(\phi) = \frac{\partial \mathcal{L}_p}{\partial \phi}$$

$$H(\phi) = \frac{\partial^2 \mathcal{L}_p}{\partial \phi^2}$$

Starting from an initial estimate $\phi^{(0)}$, solve iteratively using the **Newton-Raphson** method, with:

$$\phi^{(i+1)} = \phi^{(i)} - H(\phi^{(i)})^{-1} J(\phi^{(i)})$$

This method is integrated with smoothing parameter (λ) selection

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Discussion

Interesting method with several **potential applications**

(Relatively) complex estimation and computational techniques

Comparison of **linear constrained** and **non-linear unconstrained** optimization

Shape constrained additive models fully implemented in the R package `scam`



Extensions

Framework already extended to **bi-dimensional risk surfaces** through a tensor product basis functions

Not easy to address the original problem that motivated the research:
shape-constrained exposure-lag-response functions