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Shape-constrained splines

Applications and examples in R

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Centre for Statistical Methodology – LSHTM 30 October 2015

Gasparrini & Chalabi Shape-constrained splines

Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions
Outlin	пе				
•	Splines in reį	gression models			
2 [Defining con	straints to the s	hape		
3 9	Shape consti	rained additive n	nodels		
4 9	Some examp	les in R			
5	Extensions a	nd discussion		LC SC H &J M	DNDON HOOLØ YGIENE EDICINE
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Shape-constrained splines

Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions
Outlin	пе				
1 9	oplines in r	egression models			
21		onstraints to the s	hape		
10		strained additive n	nodels		
	ome exam	nples in R			
	Extensions	and discussion			DNDON HOOLØ
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Shape-constrained splines

Scatterplot of x and y





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True relationship



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B-spline regression

The relationship between the predictor x_i and the response y_i , with i = 1, ..., 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 $x_1 \le x \le x_n$:

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

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



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Spline basis terms

Splines



Shape-constrained splines

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Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions

Estimation

By defining:

$$\boldsymbol{\gamma} = [\gamma_1, \dots, \gamma_k, \dots, \gamma_m]^\mathsf{T} \\ \mathbf{x}_i = [b_{1,r}(x_i), \dots, b_{k,r}(x_i), \dots, b_{m,r}(x_i)]^\mathsf{T}$$

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

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



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Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions

Splines and coefficients





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Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions
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Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions
Com	parison				





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Issues and motivation

Two issues:

- 'Wiggly' shape: need to define optimal smoothness of the curve [NB: discussed in a previous CSM seminar]
- 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



Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions

Outline



(2) Defining constraints to the shape



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Derivatives of a spline function

For a B-spline function:

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

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

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

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



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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, ..., m

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



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Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions

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:

$$egin{array}{ll} f'(x;m{\gamma})>0&\Rightarrow& \mathbf{D}_1m{\gamma}>\mathbf{0}\ f''(x;m{\gamma})>0&\Rightarrow& \mathbf{D}_2m{\gamma}>\mathbf{0} \end{array}$$



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Type of constraints

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

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



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Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions

Outline

Splines in regression models

2 Defining constraints to the shape

3 Shape constrained additive models

Some examples in R

Extensions and discussion



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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:

- 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**



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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, ..., m

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

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



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Matrix formulation

Setting
$$\boldsymbol{\gamma} = \mathbf{P} \tilde{\phi}$$
, with $\tilde{\phi} = [\phi_1, e^{\phi_2}, \dots, e^{\phi_m}]^T$, and
$$\mathbf{P} = \begin{pmatrix} \begin{smallmatrix} 1 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & 1 & \cdots & 1 \end{pmatrix}$$

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

$$f(x;\phi) = \mathbf{XP} ilde{\phi}$$

Fitted through non-linear unconstrained optimization



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Shape constrained penalized splines

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

The least square objective can be modified to:

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

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



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Maximizing the log-likelihood

$$\mathcal{L}_{p}(\phi, \lambda) = \mathcal{L}(\phi) - \frac{1}{2}\lambda\phi^{\mathsf{T}}\mathbf{S}\phi$$
$$J(\phi) = \frac{\partial\mathcal{L}_{p}}{\partial\phi}$$
$$H(\phi) = \frac{\partial^{2}\mathcal{L}_{p}}{\partial\phi^{2}}$$

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





Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions
Outlin					
Outin	le				
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21	Defining co	nstraints to the s	hape		
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Outline	Splines	Shape-constraints	Shape-constraints	R examples	Extensions
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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



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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



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