Smoothing splines for densities

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Outline

clr transformation

Goal: to perform FDA exploiting the efficient routines available in L^2 space (i.e. avoid computations in Bayes spaces)

- isometric isomorphism between $\mathcal{B}^2(I)$ and $L^2(I)$

$$\mathrm{clr}(f)(x) := \ln f(x) - \frac{1}{\eta}\int_I \ln f(y)\,\mathrm{d}y$$

  and we will use notation $f_c(x) = \mathrm{clr}(f)(x)$

- operations and inner product

$$\mathrm{clr}(f \oplus g)(x) = f_c(x) + g_c(x), \qquad \mathrm{clr}(\alpha \odot f)(x) = \alpha \cdot f_c(x)$$

$$\langle f, g\rangle_{\mathcal{B}} = \langle f_c, g_c\rangle_2 = \int_I f_c(x) g_c(x)\,\mathrm{d}x$$

clr transformation

- clr transformation of density leads to the change of integral constraint

$$\int_I f(x)\mathrm{d}x = 1 \qquad \rightarrow \qquad \int_I \mathrm{clr}(f)(x)\mathrm{d}x = 0$$

$\Rightarrow$ for clr-transformed density with zero integral we have clr space $L_0^2(I)$

- inverse clr transformation is obtained as

$$\mathrm{clr}^{-1}[f_c(x)] = \frac{\exp(f_c(x))}{\int_I \exp(f_c(y))\,\mathrm{d}y}$$

The basic idea

How to approximate density function $f(x)$ by using spline?

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$$f(x) \in \mathcal{B}^2(I) \xrightarrow{\text{clr}}$$

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$$f(x) \in \mathcal{B}^2(I) \xrightarrow{\text{clr}} f_c(x) \in L_0^2(I)$$

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$$f(x) \in \mathcal{B}^2(I) \xrightarrow{\text{clr}} f_c(x) \in L_0^2(I)$$

$$\Big\downarrow \text{spline approximation}$$

The basic idea

How to approximate density function $f(x)$ by using spline?

$$
\begin{array}{ccc}
f(x) \in \mathcal{B}^2(I) & \xrightarrow{\text{clr}} & f_c(x) \in L_0^2(I) \\
 & & \Big\downarrow \text{spline approximation} \\
 & & s_k(x) \in \mathcal{S}_k^{\Delta\lambda}(I)
\end{array}
$$

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How to approximate density function $f(x)$ by using spline?

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f(x) \in \mathcal{B}^2(I) & \xrightarrow{\text{clr}} & f_c(x) \in L_0^2(I) \\
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\xi_k(x) \in \mathcal{C}_k^{\Delta\lambda}(I) & \xleftarrow[\text{clr}^{-1}]{} & s_k(x) \in \mathcal{S}_k^{\Delta\lambda}(I)
\end{array}
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The basic idea

How to approximate density function $f(x)$ by using spline?

$$\begin{array}{ccc} f(x) \in \mathcal{B}^2(I) & \xrightarrow{\text{clr}} & f_c(x) \in L_0^2(I) \\ & & \big\downarrow \text{spline approximation} \\ \xi_k(x) \in \mathcal{C}_k^{\Delta\lambda}(I) & \xleftarrow[\text{clr}^{-1}]{} & s_k(x) \in \mathcal{S}_k^{\Delta\lambda}(I) \end{array}$$

Compositional spline $\xi_k(x)$ approximates $f(x)$ in $\mathcal{B}^2(I)$.

The basic idea *updated*

How to approximate density function $f(x)$ by using spline?

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\begin{array}{ccc}
f(x) \in \mathcal{B}^2(I) & \xrightarrow{\text{clr}} & f_c(x) \in L_0^2(I) \\
 & & \big\downarrow \text{spline approximation} \\
\xi_k(x) \in \mathcal{C}_k^{\Delta\lambda}(I) & \xleftarrow[\text{clr}^{-1}]{} & s_k(x) \in \mathcal{Z}_k^{\Delta\lambda}(I)
\end{array}
$$

Compositional spline $\xi_k(x)$ approximates $f(x)$ in $\mathcal{B}^2(I)$.

Spline functions

Classical sources

- C. de Boor: *A practical guide to splines*. Applied Mathematical Sciences. Vol. 27, Springer, New York, 1978.
- L. L. Schumaker: *Spline functions: basic theory*. Wiley, New York, 1981.

Using in approximation theory

- P. Dierckx: *Curve and surface fitting with splines*. Oxford University Press, New York, 1993.

Spline as a linear combination of *B*-splines

- sequence of knots

$$(\Delta\lambda): \ \lambda_0 = a < \lambda_1 < \ldots < \lambda_g < b = \lambda_{g+1}$$

- $\mathcal{S}_k^{\Delta\lambda}[a, b]$ - the vector space of polynomial splines of degree $k > 0$, defined on a finite interval $[a, b]$ with the given sequence of knots $\Delta\lambda$ and

$$dim\, \mathcal{S}_k^{\Delta\lambda}[a, b] \ = \ g + k + 1$$

- *B*-splines basis functions $B_i^{k+1}(x)$ in $\mathcal{S}_k^{\Delta\lambda}[a, b]$
- additional knots

$$\lambda_{-k} \leq \cdots \leq \lambda_{-1} \leq \lambda_0 = a, \quad b = \lambda_{g+1} \leq \lambda_{g+2} \leq \cdots \leq \lambda_{g+k+1}$$

Spline as a linear combination of B-splines

- every spline $s_k(x) \in \mathcal{S}_k^{\Delta\lambda}[a, b]$ has a unique representation

$$s_k(x) = \sum_{i=-k}^{g} b_i B_i^{k+1}(x)$$

- using matrix notation

$$s_k(x) = \mathrm{B}_{k+1}(x)\mathrm{b}$$

where $\mathrm{b} = (b_{-k}, \cdots, b_g)^\top$ is vector of B-spline coefficients
$\mathrm{B}_{k+1}(x) = \left(B_{-k}^{k+1}(x), \cdots, B_g^{k+1}(x)\right)$ is collocation matrix

Task

- given data (x_i, y_i), $i = 1, \ldots, n$, weights $w_i > 0$, parameter $\alpha \in (0, 1)$
- find spline $s_k(x) \in \mathcal{S}_k^{\Delta\lambda}[a, b]$ such that minimizes functional

$$J_l(f) = (1-\alpha) \int_a^b \left[f^{(l)}(x)\right]^2 dx + \alpha \sum_{j=1}^{n} w_j \left[y_j - f(x_j)\right]^2$$

for $l \in \{0, 1, \ldots, k-1\}$

J. Machalová: *Optimal interpolatory and optimal smoothing splines*, Journal of Electrical Engineering 53 (12/s), 79-82, 2002.

Approximation of clr-transformed density function

Find spline $s_k(x) \in \mathcal{S}_k^{\Delta\lambda}[a,b]$ such that minimizes functional

$$J_l(s_k) = (1-\alpha)\int_a^b \left[s_k^{(l)}(x)\right]^2 dx + \alpha \sum_{j=1}^{n} w_j \left[y_j - s_k(x_j)\right]^2$$

and which satisfies an additional constraint

$$\int_a^b s_k(x)\,\mathrm{d}x = 0.$$

J. Machalová, K. Hron, G.S. Monti.: *Preprocessing of centred logratio transformed density functions using smoothing splines*, Journal of Applied Statistics 43 (8), 1419–1435, 2016.

Matrix notation

Let us denote $\mathrm{x} = (x_1, \ldots, x_n)^\top$, $\mathrm{y} = (y_1, \ldots, y_n)^\top$, $\mathrm{w} = (w_1, \ldots, w_n)^\top$ and $\mathrm{W} = diag\,(\mathrm{w})$.

Then functional $J_l(s_k)$ can be written in a matrix form as

$$J_l(\mathrm{b}) \;=\; (1-\alpha)\mathrm{b}^\top \mathrm{N}_{kl}\mathrm{b} + \alpha\,[\mathrm{y} - \mathrm{B}_{k+1}(\mathrm{x})\mathrm{b}]^\top\, \mathrm{W}\,[\mathrm{y} - \mathrm{B}_{k+1}(\mathrm{x})\mathrm{b}]$$

where

- N_{kl} is positive semidefinite matrix which is known,
- $\mathrm{B}_{k+1}(\mathrm{x}) \;=\; \left(B_i^{k+1}(x_j)\right)_{i=-k,\, j=1}^{g,n}$ is collocation matrix,
- $\mathrm{b} = (b_{-k}, \ldots, b_g)^\top$ is unknown vector of B-spline coefficients.

Integral constraint

With coincident additional knots we have

$$0 = \int_a^b s_k(x)\,\mathrm{d}x = [s_{k+1}(x)]_a^b = s_{k+1}(\lambda_{g+1}) - s_{k+1}(\lambda_0) = c_g - c_{-k-1},$$

where

$$s_{k+1}(x) = \sum_{i=-k-1}^{g} c_i B_i^{k+2}(x),$$

and

$$b_i = (k+1)\,\frac{c_i - c_{i-1}}{\lambda_{i+k+1} - \lambda_i} \quad \forall i = -k, \ldots, g.$$

Then

$$\boxed{c_{-k-1} = c_g.}$$

Finding optimal smoothing spline with zero integral

- we have relation $\mathrm{b} = \mathrm{DK}\bar{\mathrm{c}}$ with known matrix D, K
- by replacing in $J_l(\mathrm{b})$ we have $J_l(\bar{\mathrm{c}})$

$$J_l(\bar{\mathrm{c}}) = (1-\alpha)\left(\mathrm{DK}\bar{\mathrm{c}}\right)^{\top}\mathrm{N}_{kl}\mathrm{DK}\bar{\mathrm{c}} + \\ + \alpha\left[\mathrm{y} - \mathrm{B}_{k+1}(\mathrm{x})\mathrm{DK}\bar{\mathrm{c}}\right]^{\top}\mathrm{W}\left[\mathrm{y} - \mathrm{B}_{k+1}(\mathrm{x})\mathrm{DK}\bar{\mathrm{c}}\right]$$

- optimization problem without constraint
- solution

$$\bar{\mathrm{c}}^* = \alpha\,\mathrm{A}^{-}\mathrm{K}^{\top}\mathrm{D}^{\top}\mathrm{B}_{k+1}^{\top}(\mathrm{x})\mathrm{W}\mathrm{y}$$

with

$$\mathrm{A} = (1-\alpha)\left(\mathrm{DK}\right)^{\top}\mathrm{N}_{kl}\,\mathrm{DK} + \alpha\left(\mathrm{B}_{k+1}(\mathrm{x})\mathrm{DK}\right)^{\top}\mathrm{W}\,\mathrm{B}_{k+1}(\mathrm{x})\mathrm{DK}$$

- finally $\mathrm{b}^* = \mathrm{DK}\bar{\mathrm{c}}^*$

Basis functions in L_0^2

ZB-**splines** - basis functions with zero integral

Let the functions $Z_i^{k+1}(x)$ for $k \geq 0$ be defined

$$Z_i^{k+1}(x) := \frac{\mathrm{d}}{\mathrm{d}x} B_i^{k+2}(x)$$

$$Z_i^1(x) = \begin{cases} 1 & \text{if } x \in [\lambda_i, \lambda_{i+1}) \\ -1 & \text{if } x \in (\lambda_{i+1}, \lambda_{i+2}] \end{cases}$$

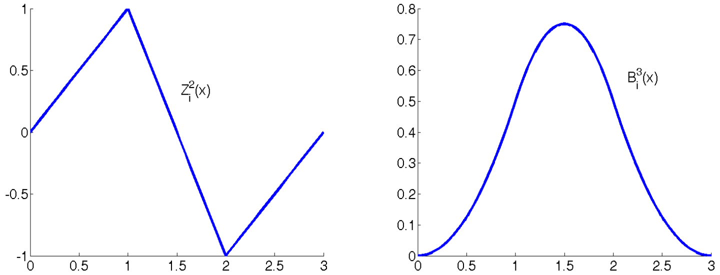
and for $k \geq 1$

$$Z_i^{k+1}(x) = (k+1) \left(\frac{B_i^{k+1}(x)}{\lambda_{i+k+1} - \lambda_i} - \frac{B_{i+1}^{k+1}(x)}{\lambda_{i+k+2} - \lambda_{i+1}} \right).$$

Example of ZB-spline

Example 1

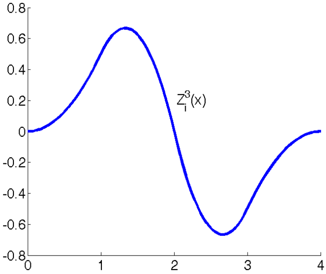
linear ZB-spline $Z_i^2(x) = \frac{\mathrm{d}}{\mathrm{d}x} B_i^3(x)$ with equidistant knots $0, 1, 2, 3$.

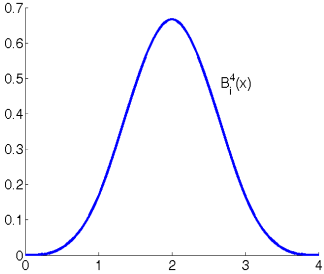


Example of *ZB*-spline

Example 2

quadratic *ZB*-spline $Z_i^3(x) = \frac{\mathrm{d}}{\mathrm{d}x} B_i^4(x)$ with equidistant knots $0, 1, 2, 3, 4$

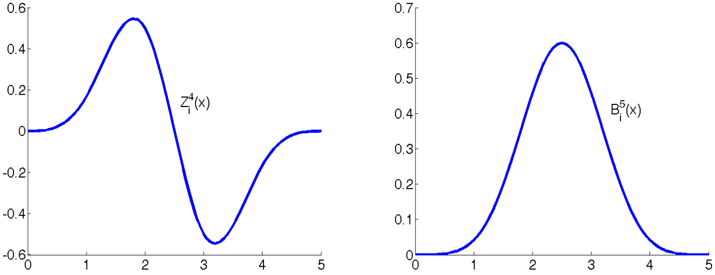




Example of ZB-spline

Example 3

cubic ZB-spline $Z_i^4(x) = \frac{\mathrm{d}}{\mathrm{d}x} B_i^5(x)$ with equidistant knots $0, 1, 2, 3, 4, 5$.



Properties of ZB-splines

- $Z_i^{k+1}(x)$ have similar properties as B-splines $B_i^{k+1}(x)$
- let $\mathcal{Z}_k^{\Delta\lambda}[a,b]$ denote the space of polynomial splines of degree $k>0$, defined on a finite interval $[a,b]$ with the sequence of knots $\Delta\lambda$ and having zero integral on $[a,b]$
- $\dim\left(\mathcal{Z}_k^{\Delta\lambda}[a,b]\right) = g+k$
- $Z_{-k}^{k+1}(x),\cdots,Z_{g-1}^{k+1}(x)$ are basis functions
- every spline $s_k(x)\in\mathcal{Z}_k^{\Delta\lambda}[a,b]$ has a unique representation

$$s_k\left(x\right)=\sum_{i=-k}^{g-1} z_i Z_i^{k+1}\left(x\right)$$

Comparison

Both ways are possible because of

Theorem

Every spline $s_k(x) \in \mathcal{Z}_k^{\Delta\lambda}[a, b]$, $s_k(x) = \sum_{i=-k}^{g-1} z_i Z_i^{k+1}(x)$ *is an element of the space* $\mathcal{S}_k^{\Delta\lambda}[a, b]$ *and fulfils the condition* $\int_a^b s_k(x)\, dx = 0$.

But now we can use basis functions with zero integral on $[a, b]$!

Matrix representation

$s_k(x) = \sum_{i=-k}^{g-1} b_i Z_i^{k+1}(x)$ can be written in matrix notation

$$s_k(x) = \mathrm{Z}_{k+1}(x)\mathrm{z}$$

where

$$\mathrm{Z}_{k+1}(x) = \left(Z_{-k}^{k+1}(x), \ldots, Z_{g-1}^{k+1}(x)\right)$$

and

$$\mathrm{z} = \left(z_{-k}, \ldots, z_{g-1}\right)^{\top}$$

Relationship

By using notation

$$\mathrm{B}_{k+1}(x) = (B_{-k}^{k+1}(x), \dots, B_{g}^{k+1}(x))$$

we can write

$$\mathrm{Z}_{k+1}(x) \ = \ \mathrm{B}_{k+1}(x)\mathrm{DK}$$

where D is a diagonal matrix dependent on knots
K is a matrix with two nonzero diagonals of elements ± 1 then

$$s_k(x) \ = \ \mathrm{B}_{k+1}(x)\mathrm{DKz}$$

Finding optimal smoothing spline with zero integral

Task: to find a spline $s_k(x) \in \mathcal{Z}_k^{\Delta\lambda}[a,b]$ which minimizes $J_l(s_k)$

- in matrix notation (in a simplified way)

$$J_l(\mathrm{z}) = \mathrm{z}^\top \mathrm{G}\mathrm{z} - 2\mathrm{z}^\top \mathrm{g} + \alpha \mathrm{y}^\top \mathrm{W}\mathrm{y}$$

- its minimum is

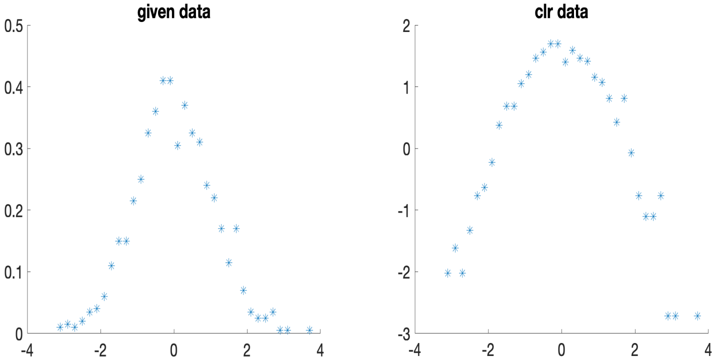
$$\mathrm{z}^* = \mathrm{G}^{-1}\mathrm{g}$$

- the resulting smoothing spline is obtained by formula

$$s_k^*(x) = \sum_{i=-k}^{g-1} z_i^* Z_i^{k+1}(x), \qquad s_k^*(x) = \mathrm{B}_{k+1}(x)\mathrm{D}\mathrm{K}\mathrm{z}^*$$

Example - simulation from normal distribution

For optimal smoothing spline we use $k = 2$, $l = 1$, $w_i = 1 \, \forall i$, $\alpha = 0.5$



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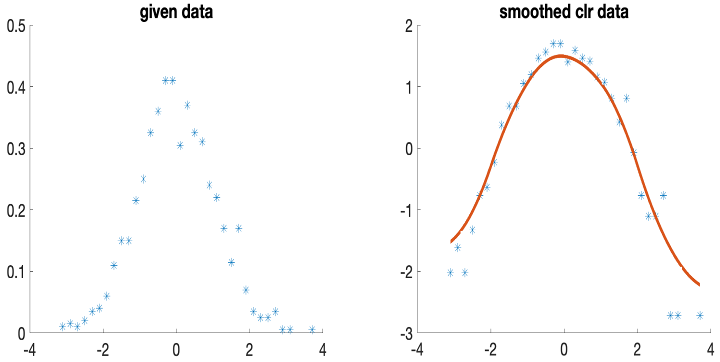

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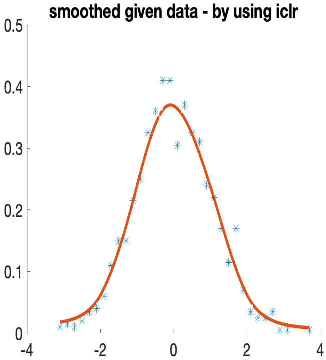

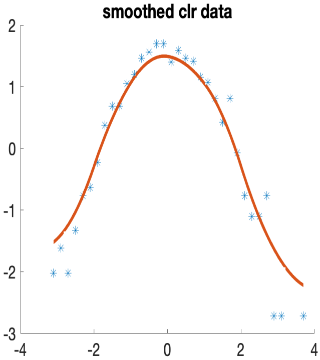

back-transformation

- we use back-transformation of B-splines from $L_0^2(I)$ to the original Bayes space $\mathcal{B}^2(I)$ for $i = -k, \ldots, g-1,\ k \geq 0$

$$\zeta_i^{k+1}(x) = \exp[Z_i^{k+1}(x)]$$

  and we call them *compositional B-splines*

- $\mathcal{C}_k^{\Delta\lambda}[a, b]$ denotes the vector space of polynomial splines of degree $k > 0$, defined on a finite interval $[a, b]$ with the sequence of knots $\Delta\lambda$
- $\dim\left(\mathcal{C}_k^{\Delta\lambda}[a, b]\right) = g + k$

Back to Bayes space

Every spline $\xi_k(x) \in \mathcal{C}_k^{\Delta\lambda}[a, b]$ in $\mathcal{B}^2(I)$ can be uniquely represented as

$$\xi_k(x) = \bigoplus_{i=-k}^{g-1} c_i \odot \zeta_i^{k+1}(x)$$

and we call it *compositional spline*.

J. Machalová, R. Talská, K. Hron, A. Gába: *Compositional splines for representation of density functions*, Computational Statistics, 2021. doi: 10.1007/s00180-020-01042-7.

compositionalSpline *Compositional spline*

Description

This code implements the compositional smoothing splines grounded on the theory of Bayes spaces.

Usage

compositionalSpline(t,clrf,knots,w,order,der,alpha,spline.plot = FALSE, basis.plot = FALSE)

Value

J	value of the functional J
ZB_coef	ZB-spline basis coefficients
CV	score of cross-validation
GCV	score of generalized cross-validation