

## Some News Regarding the Regression Splines:

- Bernstein polynomials and Least-Squares Splines.
- Variations around the identity spline function.

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## Abstract

Two distinct parts:

- A practical view on P-splines and Least-Squares splines
  - quasi-interpolation versus exact interpolation
  - adaptive smoothing versus Bernstein modeling-smoothing.

A data-poor information-rich data set (page 24):

$x$ : a sample from the uniform distribution,

$y$ : the "cornell" response, (6), (20).

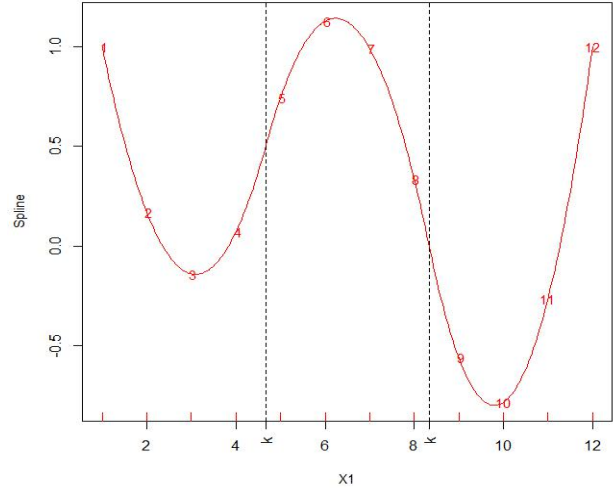
- A new functional technique to experiment with desirable changes of the response variable.
  - The tool: flexible variations around the identity spline function,
    - online local or global changes in the observations.
  - Available in any regression method,
    - here, in Boosted Partial Least-Squares models,
    - to alleviate poverty in the Italian social context.

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# 1. Splines in a nugget

A spline  $s(x)$  transforming  $x$ ,  $range(x) = [a, b]$ , is made of **adjacent polynomials** of degree  $d$ , or order  $m = d + 1$ , that join end to end at  $K$  points called **”the knots”**.



- **Zero/Few/Many (?)** knots  $\tau_j$  whose locations (if any) **inside**  $]a, b[$  and their number  $K$ , joined to the degree, are the tuning parameters.

$$\tau_1 = \dots = \tau_m = a < \tau_{m+1} \leq \dots \leq \tau_{m+K} < b = \tau_{m+K+1} = \dots = \tau_{2m+K}.$$

- **A functional linear space**  $S_{[a,b]}$  of dimension  $m + K$  whose most popular basis functions  $\{B_j^m(\cdot)\}_{j=1,\dots,m+K}$  are **the B-splines**

$$s(x, \beta) = \sum_{j=1}^{m+K} \beta_j B_j^m(x). \tag{1}$$

Here, in the first part, **the  $\beta$  coefficients are resulting from a  $L_2$  regression** as expressed in the general framework of the P-splines (9) with a **discussion on whether or not penalizing the  $L_2$  cost**.

## 2. Splines in bivariate regression

Data:  $\{\mathbf{x}, \mathbf{y}\}$ , a bivariate set of  $n$  observations. Here, data on page 24.

### 2.1 The P-splines of Eilers and Marx

To deal with the **overfitting issue** when using a **large number of equally spaced knots**, (9), (10), P-splines propose to penalize the  $L_2$  cost by a **penalty  $\lambda$  on  $k$ -finite differences of adjacent  $\beta$  coefficients**:

$$\|\mathbf{y} - \mathbf{B}\boldsymbol{\beta}\|^2 + \lambda\|\mathbf{D}_k\boldsymbol{\beta}\|^2,$$

where the  $n \times (m+K)$   $\mathbf{B}$  and  $\mathbf{D}_k$  matrices are respectively the  $B$ -splines codings of  $\mathbf{x}$  and the matrix of finite differences. So, P-splines may be considered as a finite dimensional RKHS regularization type with a discrete penalty on adjacent coefficients:

$$\mathbf{H} = \mathbf{B}(\mathbf{B}'\mathbf{B} + \lambda\mathbf{D}_k'\mathbf{D}_k)^{-1}\mathbf{B}'$$

$$\hat{\mathbf{y}} = \mathbf{H}\mathbf{y}.$$

When  $n = K$  going to infinity, P-splines lead to smoothing splines (14).

- $\lambda = 0 \longrightarrow$  **LSS, the Least-Squares Splines regression.**
- $k = 0 \longrightarrow$  **the ridge regression.**

Following (12),  $trace(\mathbf{H})$  is the effective dimension of the linear smoother  $\mathbf{H}$ , so that the Generalized Cross-Validation index

$$GCV(\lambda, k) = \frac{var(Residuals)}{(1 - trace(\mathbf{H}/n))^2}$$

is a surrogate to the Predicted Residual Error Sum of Squares (PRESS) from cross-validation.

## 2.2 Interpolation, smoothing and modeling

- $\lambda=0$  : degree, number and location of knots ( $m + K \leq n$ ).

The curse of dimensionality:  $m + K > n$ .

- $\lambda > 0$  : irrelevant knots choice for smoothing: "d = 3, many knots and a strong penalty, to provide robust and efficient smoothing".

### Interpolation

- **LSS: exact interpolation tool** with following parameters:

degree  $d \geq 1$ , the **largest admissible number of distinct knots**

$$K = n - m \implies var(Residuals) = 0$$

Drawback:  $d > 1$  erratic oscillations.

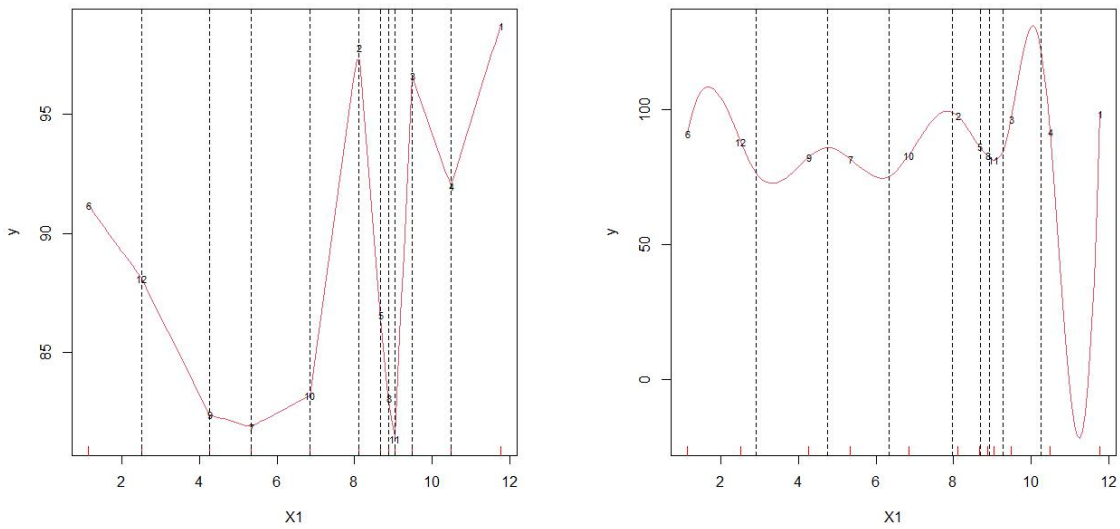
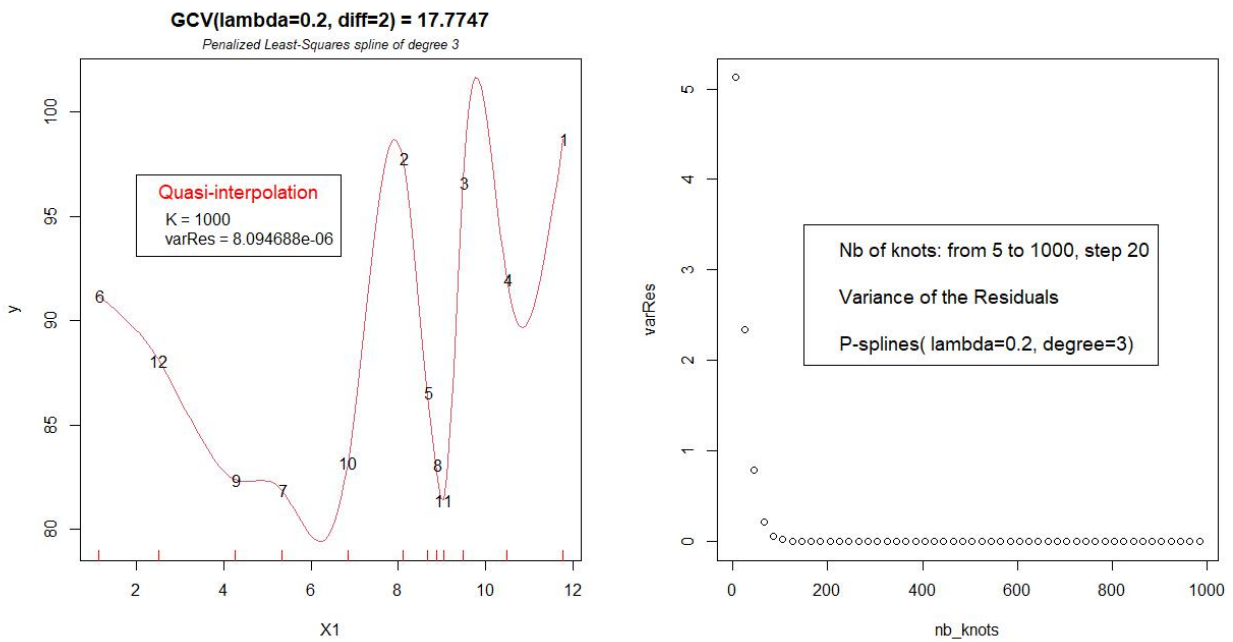


Figure 1: Exact LSS interpolation with knots at quantiles,  $d=1, K=10$  and  $d=3, K=8$ .

- **P-splines: non-erratic quasi-interpolation** (very large  $K, k = 2$ ).

$\lambda$  constrains the local curvature and  $\lim_{K \rightarrow \infty} \text{var}(\text{Residuals}) = 0$ .

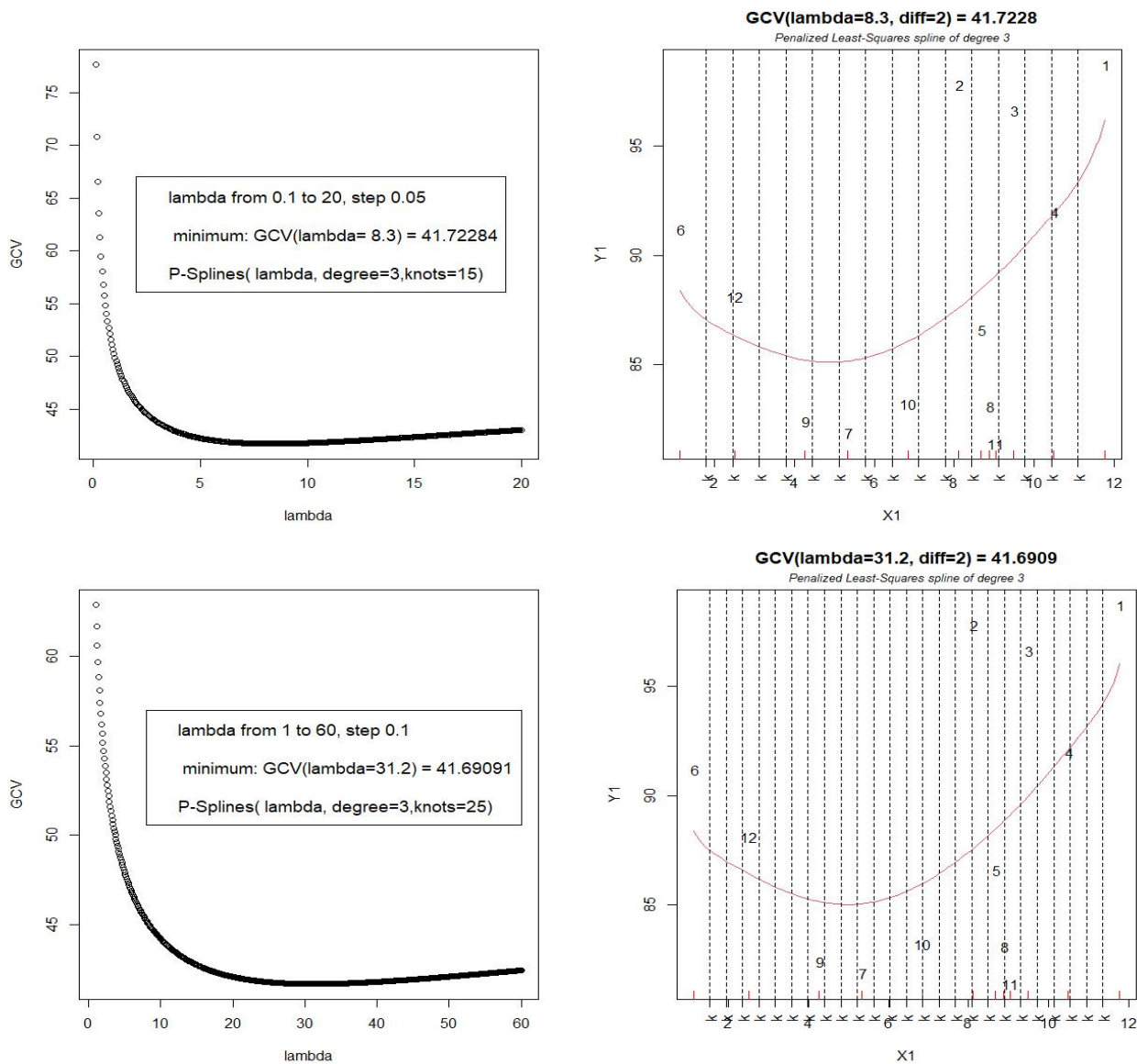
$k = 2, d = 3, \lambda = 0.2, K = 1000, \text{var}(\text{Residuals}) = 8.094688 e-06$ .



## Adaptive-smoothing/Modeling-smoothing: P-splines/LSS

### P-splines for $\lambda$ -adaptive smoothing

Two  $\{\lambda > 0, GCV(\lambda)\}$  P-splines campaigns based on 15 and 25 knots,



respectively reveal the best  $\lambda$  values 8.3 and 31.2

$$GCV(K = 15, \lambda = 8.3) = 41.7228$$

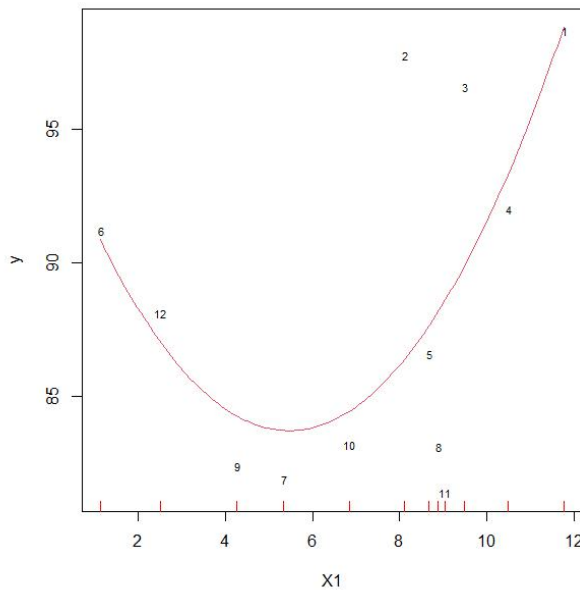
$$GCV(K = 25, \lambda = 31.2) = 41.6909$$

## LSS for modeling-smoothing

$\{\lambda = 0, K = 0\}$ : Bernstein polynomial modeling (see Section 3).

**No knots, degree 2**, revealing a **5% better GCV** of a quadratic signal,

$$LSS(K=0, d=2) \quad GCV(K = 0, d = 2) = 39.43105.$$



**LSS modeling-smoothing:**

**$LSS(K = 0, d)$  initial step.** Adding a knot increases the local flexibility of the spline and thus the freedom to fit the data in that region.

**The practice in short:**

**P-splines** ( $\lambda > 0$ ):

- A **robust adaptive smoothing tool** to deal with the overfitting issue,
- **Non-erratic quasi-interpolation:** very large number of knots.

## LSS:

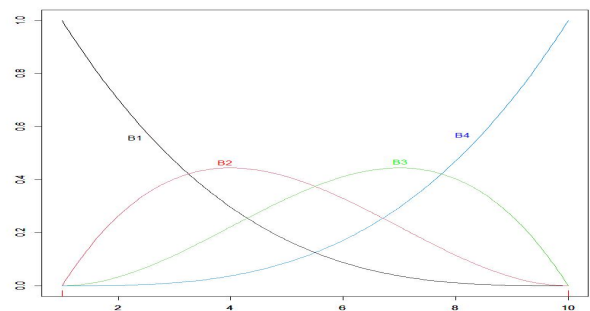
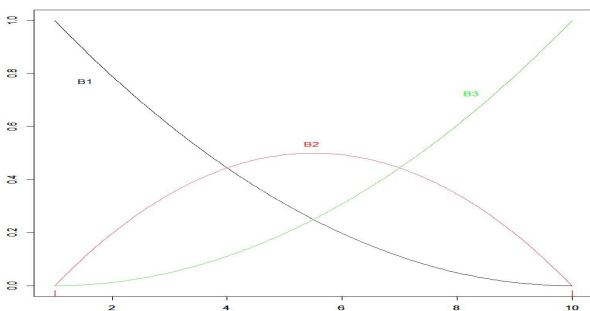
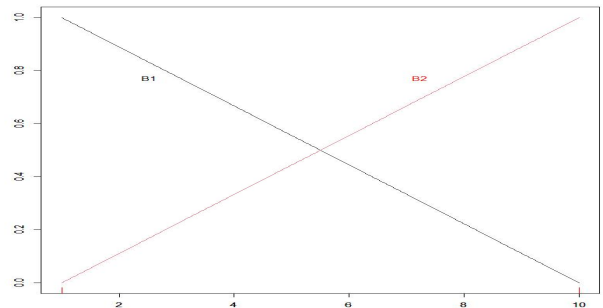
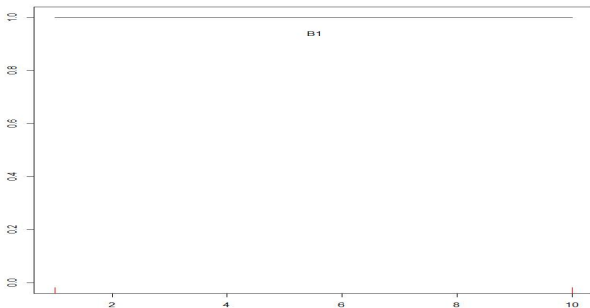
- **Non-robust**: two identical  $x$ -observations make  $B'B$  non-invertible (but, two distinct respective  $y$ -values contradict a functional signal).

Controlled curse of dimensionality,  $(m + K \leq n)$ . Even in the multivariate case by Partial Least-Squares Splines, PLSS, (5).

- **Exact interpolation** (erratic when  $d > 1$ ):  $K = n - m$  distinct knots,
- **Modeling-smoothing diversity**: polynomials, e.g. linear models, eventual smoothing by "few well located knots", discontinuities...

### 3. Main $B$ -splines properties

- **P0**:  $B$ -splines with  $K = 0$  are Bernstein polynomials on  $[a, b]$ .



– **LSS( $d, K = 0$ ) proposes polynomials as candidate models:**

$$d = 1: \text{Bernstein basis} = \left( B_1^2(x) = \frac{b-x}{b-a}, B_2^2(x) = \frac{x-a}{b-a} \right).$$

$(a_0, a_1)$  being the weights in the canonical basis  $(1, x)$ ,

$$\text{the matrix basis change: } \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \frac{1}{b-a} \begin{bmatrix} b & -a \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix}.$$

$d = 2$ :

$$\left( B_1^3(x) = \frac{(b-x)^2}{(b-a)^2}, B_2^3(x) = \frac{2(x-a)(b-x)}{(b-a)^2}, B_3^3(x) = \frac{(x-a)^2}{(b-a)^2} \right).$$

$(a_0, a_1, a_2)$ : the weights in the canonical basis  $(1, x, x^2)$ ,

$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \frac{1}{(b-a)^2} \begin{bmatrix} b^2 & -2ab & a^2 \\ -2b & 2(a+b) & -2a \\ 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}.$$

– **P-splines and polynomials:**

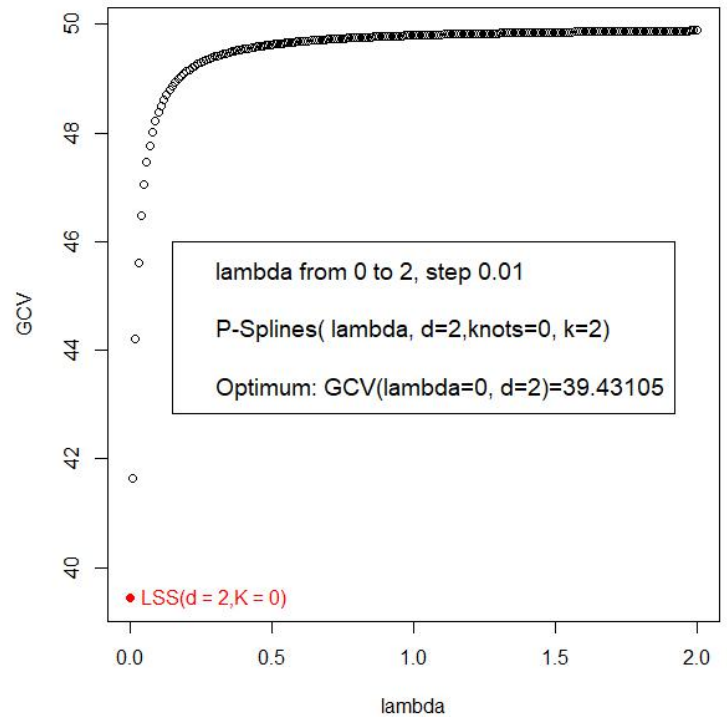
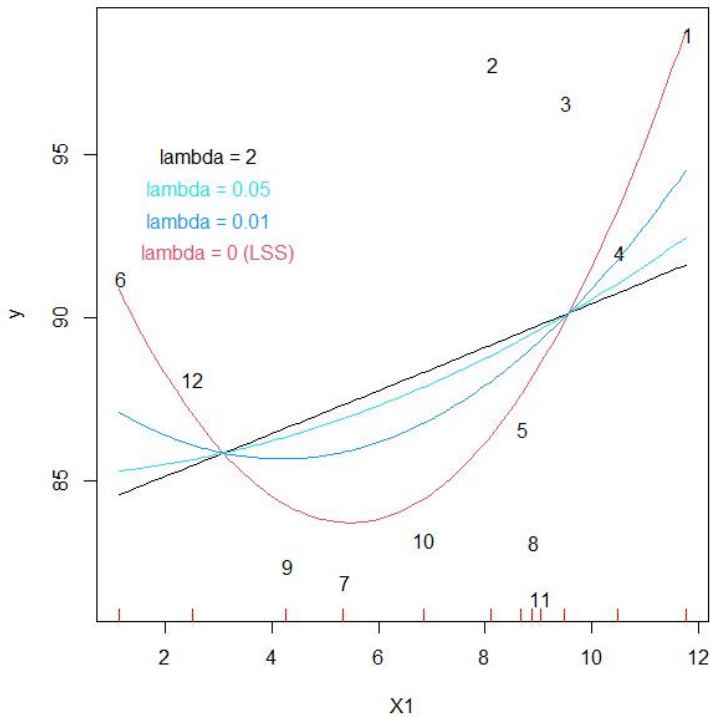
- $\lambda \rightarrow +\infty$ , a theoretical asymptotic property (2):

finite difference of order  $k$  leads to a polynomial of degree  $k - 1$ .

- **P-splines( $K = 0, d, 0 \leq k \leq d, \lambda > 0$ ) penalizes the Bernstein coefficients.** The  $\{K = 0, d = 2, k = 2, \lambda, GCV(\lambda)\}$  P-splines

campaign below illustrates **the degree 2 → degree 1 continuum**

by more and more constraining the convexity:



- **P1: Local support**

$$B_j^m(x) = 0, \quad \forall x \notin [\tau_j, \tau_{j+m}].$$

So,  $m$  non null basis functions share the same support  $[\tau_j, \tau_{j+m}]$  that makes **LSS robust against the influence of outlying observations.**

- **P2: Fuzzy coding functions**

$$0 \leq B_j^m(x) \leq 1, \quad \text{and} \quad \sum_{j=1}^{m+K} B_j^m(x) = 1.$$

So,  $B_j^m(x_i)$  functions as a degree of membership of  $x_i$  to  $[\tau_j, \tau_{j+m}]$ .

- **P3:** The multiplicity of knots controls the smoothness

The multiplicity  $m_j$  ( $1 \leq m_j \leq m$ ) of a knot  $\tau_j$  is the number of knots that merge at the same point.

Smoothness at  $\tau_j$ :  $C^{d-m_j}$ :

$d$	$m_j$	smoothness at $\tau_j$
0	1	$C^{-1}$
1	1	$C^0$
	2	$C^{-1}$
2	1	$C^1$
	2	$C^0$
	3	$C^{-1}$
3	1	$C^2$
	2	$C^1$
	3	$C^0$
	4	$C^{-1}$

## 4. Variations around the identity spline

Here, the spline coefficients are not from a statistical regression but are decided by the user to modify the "nodal" weights denoted as  $\beta_{\text{nodal}}$  corresponding to the identity spline function, (11), (18), (19), (3) and (4).

### 4.1 Definition of the nodal weights

Whatever the knots and their multiplicity, and whatever  $d > 0$ , the nodal weights  $\beta_{\text{nodal}}$  such that

$$s(x, \beta_{\text{nodal}}) = x$$

are defined by the average of  $d$  successive knots.

$$\text{for } j \in 1, \dots, m + K, \quad [\beta_{\text{nodal}}]_j = \frac{1}{d} \sum_{k=1}^d \tau_{j+k}.$$

### 4.2 Identity spline variations. Definition and practice

The input vector  $\delta$  allows additive alterations of the nodal weights,  $\beta_{\text{nodal}} + \delta$ , that allows to control local or global, continuous or discontinuous changes in the observations (8),(17). Splines belonging to a functional linear space, a  $\delta$ -scenario leads to a  $\delta$ -spline shift of the response:

$$y(\boldsymbol{\delta}) = s(y, \boldsymbol{\beta}_{\text{nodal}} + \boldsymbol{\delta}) = s(y, \boldsymbol{\beta}_{\text{nodal}}) + s(y, \boldsymbol{\delta}) = y + s(y, \boldsymbol{\delta}).$$

In particular,  $\boldsymbol{\delta} = \mathbf{0}$  leaves the response unchanged:

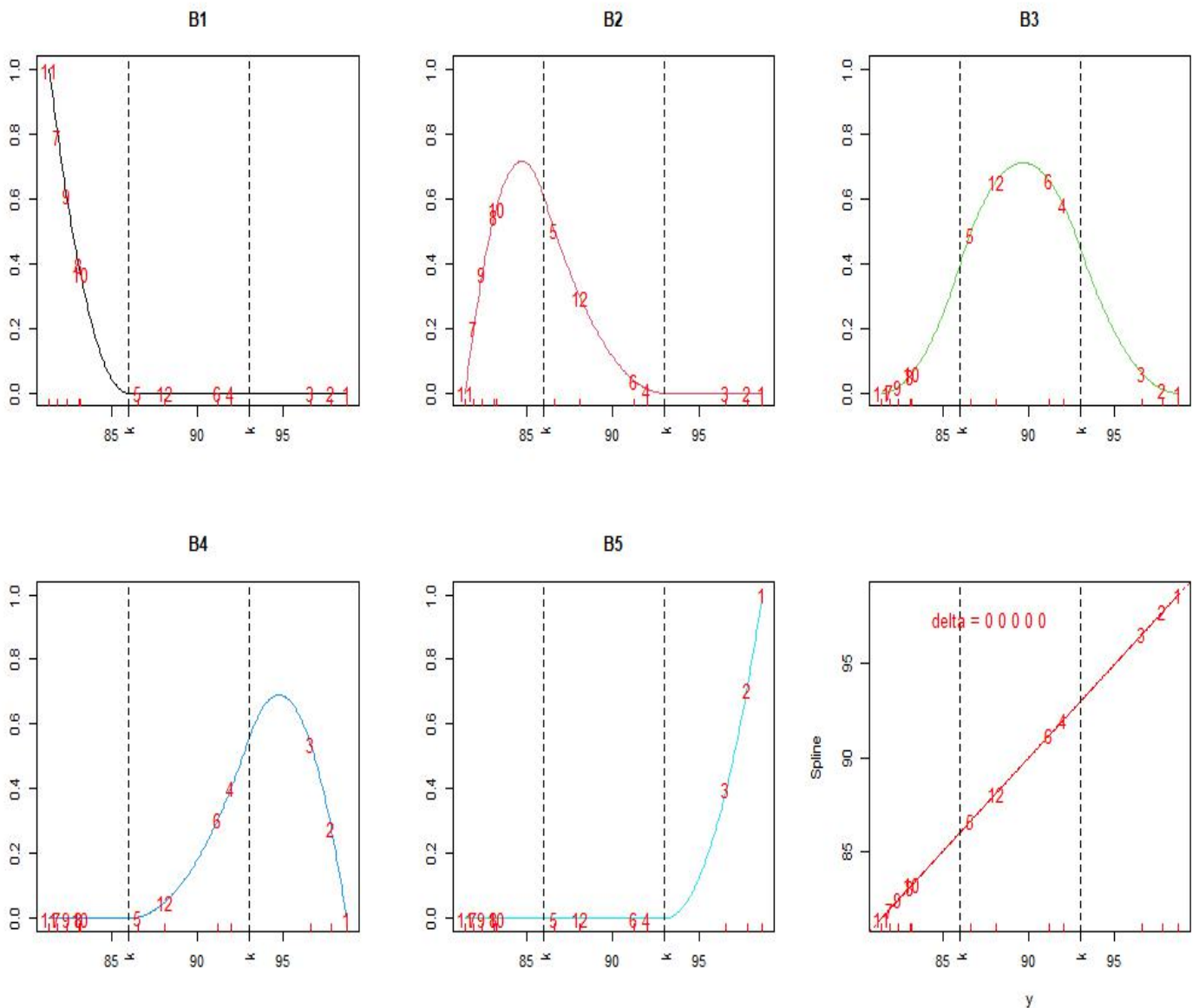


Figure 2: *B*-splines ( $d = 2$ , two knots) applied on the cornell data and the spline identity ( $\text{delta}=0$ ).

Due to **P1** and **P2**,  $m$  successive  $\delta_i = c$  on the same support, leads to a constant  $y$ -shift of  $c$ , and no local change when  $c = 0$ .

Figures	degree	knots	$\delta$ ( $length(\delta) = m + K$ )	remarks
Fig. 3	$\forall d > 0$	$\forall$ knots	constants 3 and -3	global shifts 3 and -3
Fig. 4	1	86, 93	0, 0, 3, 0	no change on $[, 86]$ shifts 0, 3 at knots
	2	86, 93	0, 0, -2.5, 0, 0	
Fig. 5	2	86, 86, 86, 93, 93, 93	1, 1, 1, -2, -2, -2, 3, 3, 3	shifts 1, -2, 3
	2	86, 86, 93, 93, 93	1, 1, -2, 5, -2, 3, 3, 3	$C^0$ at 86, $C^{-1}$ at 93

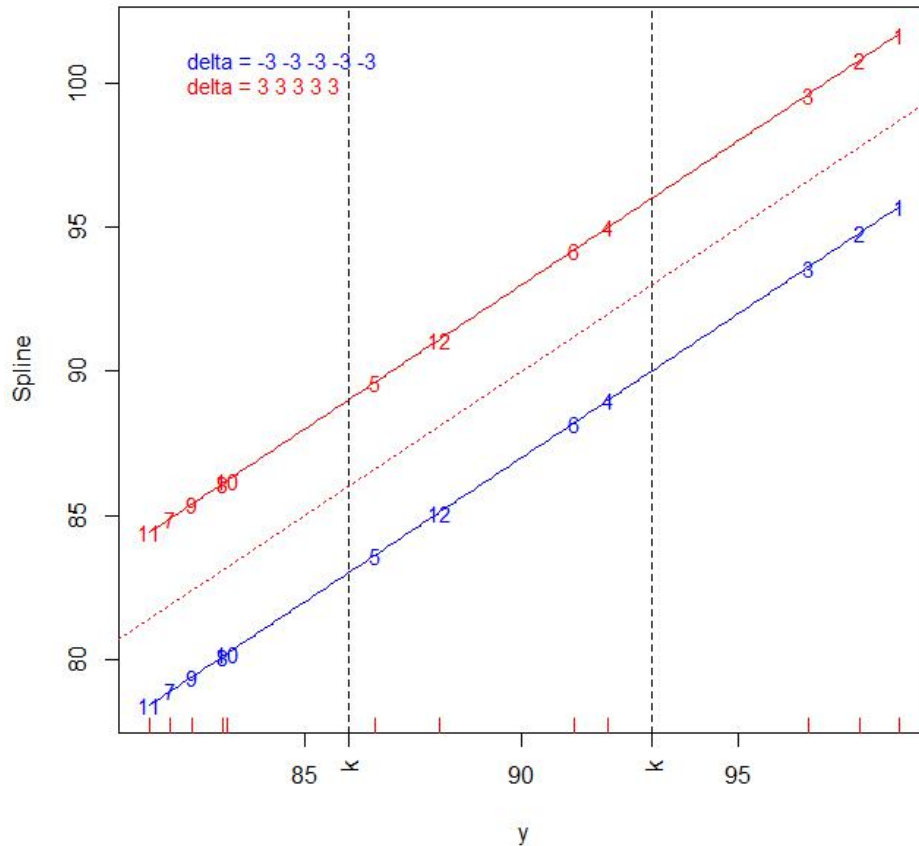


Figure 3: **Reversibility**,  $\delta = c$ ,  $\delta = -c$ , **whatever degrees and knots**, here  $d = 2$ ,  $K = 2$ : .

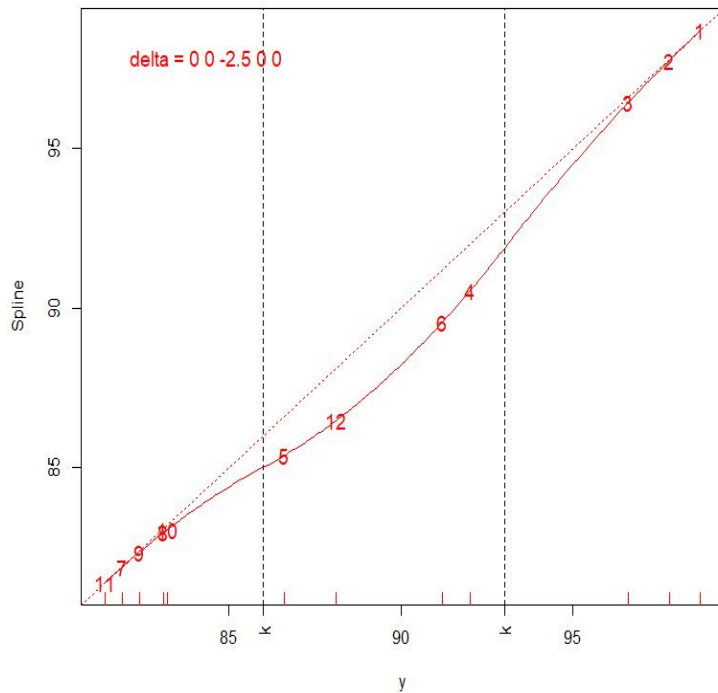
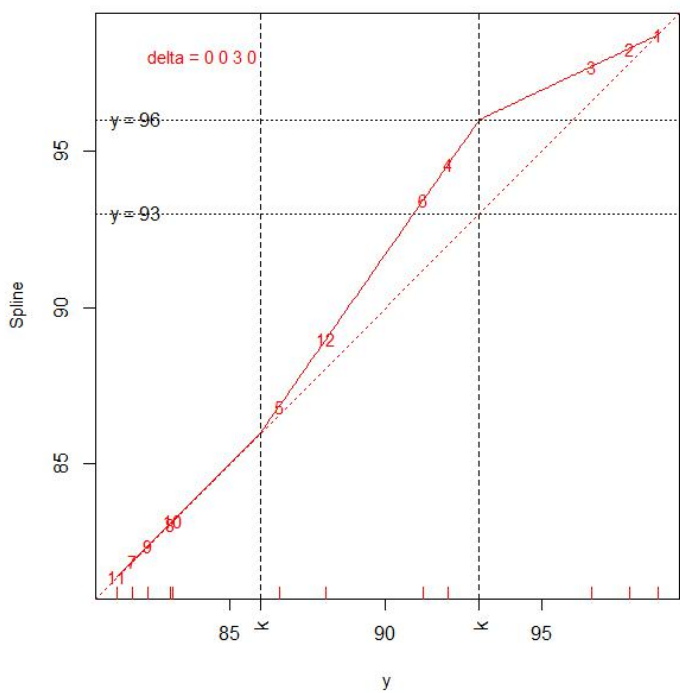


Figure 4: Degree 1 and 2, the identity spline (red dotted line), knots at 86, 93.

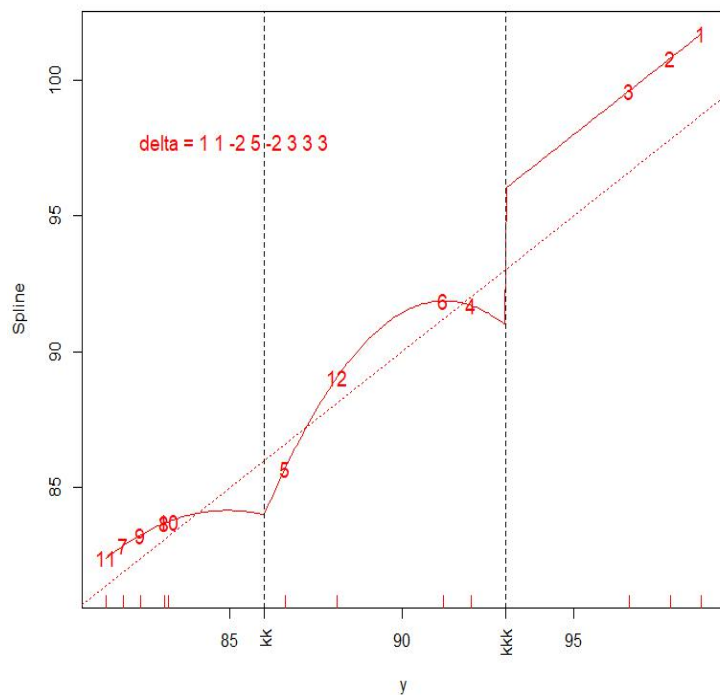
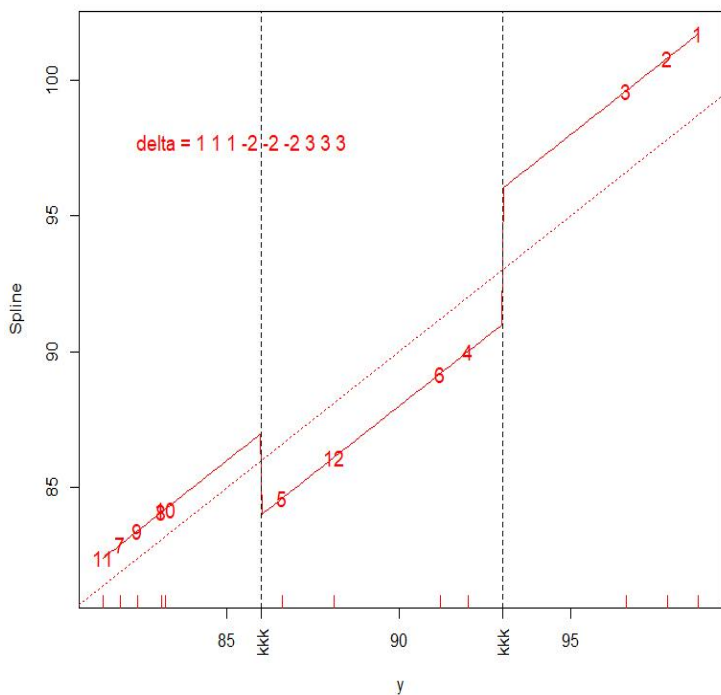


Figure 5: Degree 2 variations with multiple knots. Multiplicity is indicated by over-turned k's in  $x$ -axis labels.

## 5. Boosted Partial least-Squares regression

- $\{X = \{x_1, \dots, x_p\}, y\}$  standardized variables,  $n$  observations.
- A set of  $B$ -splines families  $B = \{B_1, \dots, B_p\}$  associated to  $X$ .
- $y(\delta)$  a selected storyboarded response. Default:  $y(\mathbf{0}) = y$ .

**PLS**: the ordinary Partial Least-Squares **linear model** (21),

**PLSS**: the Partial Least-Squares Splines model (5),

$$PLSS(X, y) = PLS(B, y).$$

- **PLSS** allows for **nonlinear and linear models** ( $P_0$ ).
- **PLS and PLSS both belong to the  $L_2$  loss boosting methods**, (1), as recursive  $L_2$  regressions of the residuals. We refer to these methods as **BPLS**, the Boosted Partial Least-Squares (7), (8).
- The estimated response linearly depends on **few  $A$  pseudo-predictors** called **the base learners**, here, **the components  $t_1, \dots, t_A$** ,

$$\hat{y}(A) = \sum_{i=1}^A \alpha_i t_i.$$

In PLSS, the generic component  $t_i$  can be expressed as

$$t_i = s_1^i(x_1) + \dots + s_p^i(x_p), \quad i = 1, \dots, A.$$

**Full dimensioned BPLS:  $A=r$** , the rank of the design matrix,

- **PLS(X,y) = OLS(X,y)** the ordinary least-squares linear model.
- $\uparrow$  **all predictors: degree = 1, no knots.**
- **PLSS(X,y) = LSS(X,y)** the multiple Least-Squares Splines model.

Avoiding the curse of dimensionality ( $A < r$ ), the best dimension  $A$  is detected by the PRESS or the GCV.

The estimated storyboarded response becomes

$$\hat{y}(\boldsymbol{\delta}, A) = \sum_{j=1}^p \sum_{l=1}^{m_j+K_j} \hat{\beta}_l^j(A) B_l^j(x_j). \quad (2)$$

- The  $p$  **coordinate functions** are **ranked in descending order** of influence **according to the range of their values.**
- A **back-pruning procedure** to eliminate those to be neglected.
- Component scatter plots are explained by linear or nonlinear coordinate spline functions.

## 5.1 Spline tuning parameters in multivariate regression

Penalized PLSS:

Inspired by the P-splines, **Kraemer et al. (13)** proposes Penalized PLSS presuming  $p$  **homogeneous** nonlinear  $(x_j, y)$  patterns.

PLSS:

A strategy to take account of **heterogeneity** in single effects:

- **Swift global option**: equally spaced knots or at quantiles.
- **Individual option**: **A preliminary look at  $\{(x_j, y)\}_{j=1}^p$  scatter plots provides informations to tailor the LSS( $x_j, y$ )-modeling to the  $p$  variables** (GCV <sub>$j$</sub>  criterion):

- **no knots** for **pure polynomials** (first try with the linear model).
- **parsimonious smoothing (few well located knots)**
- **knots multiplicity** to capture **discontinuities**,
- Possible **degree 0** for **step-shaped patterns**,

Finally, the overall validity is typically evaluated using PRESS or GCV.

## 5.2 One example of PLSS scenario to alleviate Poverty in Italia

- $X$ :  $20 \times 28$  matrix of 28 predictors observed on the 20 regions.
- $y_0$ : the observed Poverty:

$$PLS_0 = PLS(X, y_0), \quad PLSS_0 = PLSS(X, y_0).$$

- $y_1 = y(\delta)$ : the  $\delta$ -storyboarded Poverty of Figure 6 below, (8):

$$PLS_1 = PLS(X, y_1), \quad PLSS_1 = PLSS(X, y_1).$$

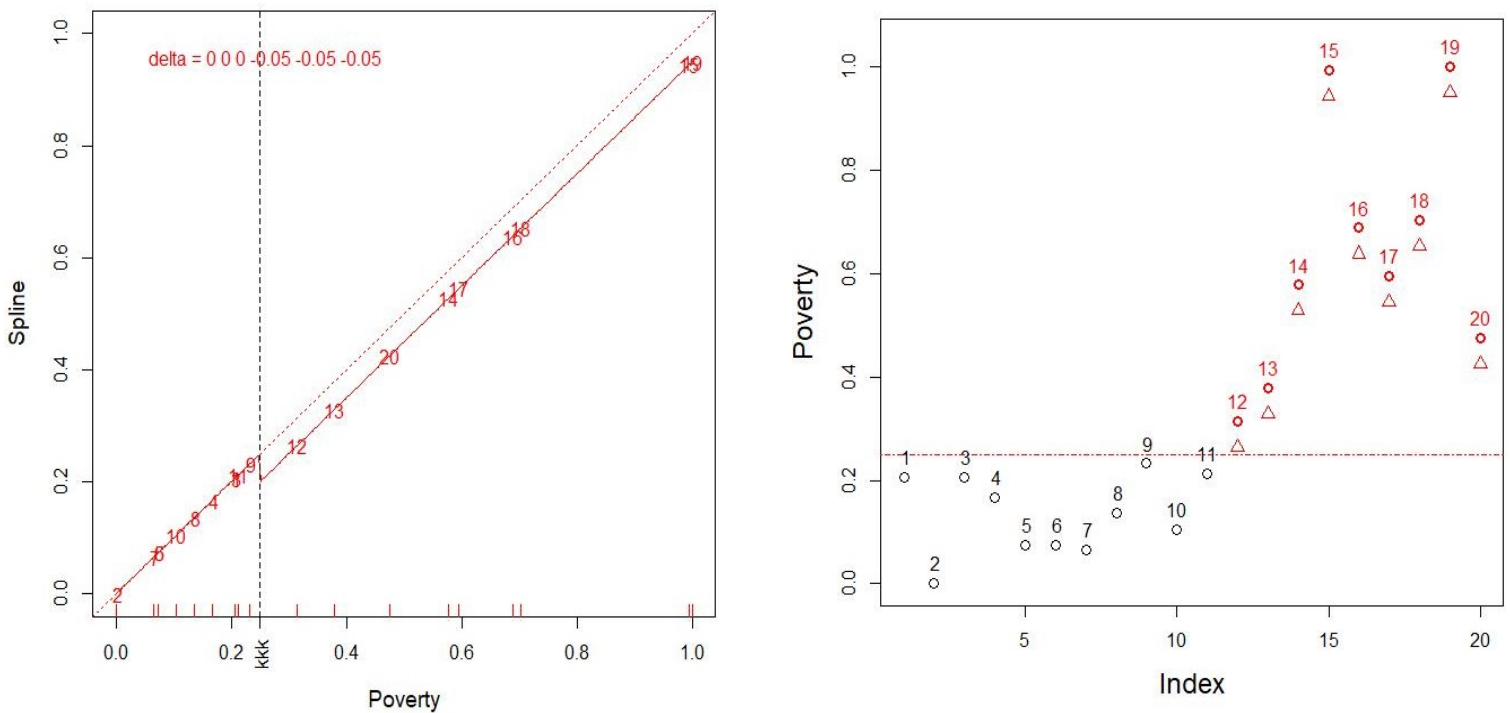


Figure 6: Degree 2, a knot of multiplicity 3 located at 0.25, the poverty average. A Poverty constant delta shift of -0.05 on the 9 most impoverished regions (in red on the right plot).

	<b>PLS<sub>0</sub></b>	<b>PLSS<sub>0</sub></b>	<b>PLS<sub>1</sub></b>	<b>PLSS<sub>1</sub></b>
<b>A</b>	4	2	2	2
<b>PRESS</b>	0.057	0.059	0.071	0.070

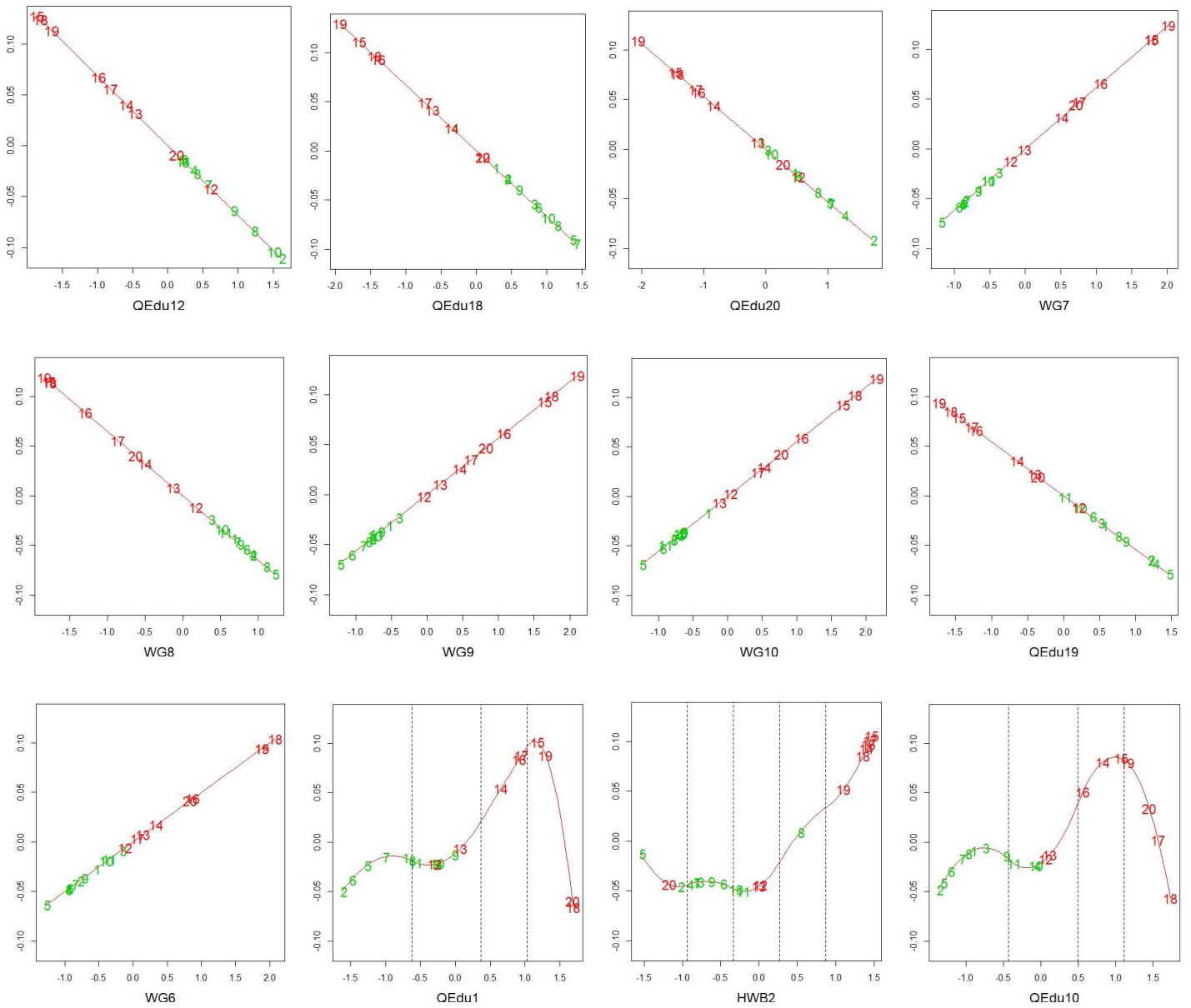


Figure 7: The storyboarded Poverty estimated by PLSS<sub>1</sub>. The 12 most influential predictors are decreasingly ordered from left to right and up to down according to the range of the coordinate functions.

Table 1: Summary of the linear and nonlinear BPLS models involving the 12 influential predictors decreasingly ordered. Notice that in PLSS, the first 9 involve linear transformations.

<b>PLS<sub>0</sub></b>	beta	<b>PLS<sub>1</sub></b>	beta	<b>PLSS<sub>0</sub></b>	range	<b>PLSS<sub>1</sub></b>	range	degree knots	
<b>HWB2</b>	0.196	QEdu12	-0.136	QEdu12	0.232	<b>QEdu12</b>	0.238	1	0
<b>HWB3</b>	0.180	HWB2	0.108	QEdu18	0.220	<b>QEdu18</b>	0.224	1	0
<b>HWB5</b>	-0.175	QEdu20	-0.107	WG8	0.196	<b>QEdu20</b>	0.220	1	0
QEdu20	-0.160	QEdu18	-0.103	WG7	0.194	WG7	0.198	1	0
QEdu12	-0.131	HWB3	0.094	QEdu20	0.189	WG8	0.198	1	0
QEdu18	-0.120	WG7	0.077	WG9	0.188	WG9	0.188	1	0
WG10	0.115	WG10	0.076	WG10	0.186	WG10	0.186	1	0
WG9	0.112	WG8	-0.074	QEdu19	0.173	QEdu19	0.173	1	0
QEdu21	0.096	WG9	0.074	WG6	0.163	WG6	0.168	1	0
WG7	0.095	WG4	0.067	QEdu1	0.158	QEdu1	0.167	2	3
QEdu7	0.089	HWB8	-0.066	HWB2	0.152	HWB2	0.156	2	4
QEdu1	0.076	QEdu19	0.063	QEdu10	0.152	QEdu10	0.141	2	3

- HWB2 :Excess weight (standardized rates). **QEdu12: Nurseries, integrated services for childhood.**
- HWB3 :Healthy life expectancy at birth. **QEdu18:Participation in continuous training.**
- HWB5:Hypertension (standardized rates). **QEdu20: Advanced digital skills.**

To alleviate the poverty in specific regions, some recommendations to modify the values of the influential predictors.

According to the scenario estimated by the PLSS<sub>1</sub> model of Figure 7:

Table 2: **In red, priorities in regions and in modifications.** The symbols have the following meaning:

- '+' or '++', for a slight or strong increase,
- '-' or '--', for a slight or strong decrease,
- '=', no change in the value of the predictor.

	QEdu12	QEdu18	QEdu20	WG7	WG8	WG9	WG10	QEdu19	WG6	QEdu1	HWB2	QEdu10
Sardegna(20)	=	=	=	-	+	-	-	+	-	=	=	--
Sicilia(19)	++	++	++	--	++	--	--	++	--	--	--	--
Calabria(18)	++	++	++	--	++	--	--	++	--	=	--	=
Basilicata(17)	+	+	+	-	+	-	-	--	=	--	--	-
Puglia(16)	+	++	+	-	++	-	--	++	--	--	--	--
Campania(15)	++	++	++	--	++	--	--	++	--	--	--	--
Molise(14)	+	+	+	-	+	-	-	+	-	-	-	--
Abruzzo(13)	+	+	=	=	=	=	=	=	=	=	=	=
Lazio(12)	=	=	=	-	+	-	=	=	=	=	=	=

## 6. Conclusion

- If one has the time to look at data,  
in competition with "ready to wear" penalties,  
"tailor made" LSS and PLSS modeling-smoothing  
allows to capture the diversity of single effects.
- To manage and evaluate projections into the future:  
a functional technique for a more desirable response  
and what changes are needed to achieve that goal.

## 7. Data sets and source files

### P-splines versus LSS bivariate R data :

```
structure(list(xrunif = c(11.7620010608807, 8.09413110627793, 9.4720985062886, 10.4787393852603,  
8.65695987828076, 1.12100960616954, 5.3243533782661, 8.86439893278293, 4.26028580009006, 6.8379231570  
9.04589922633022, 2.50727575621568), ycornell = c(98.7, 97.8, 96.6, 92, 86.6, 91.2, 81.9, 83.1, 82.4,  
83.2, 81.4, 88.1)), class = "data.frame", row.names = c("1", "2", "3", "4", "5", "6", "7", "8", "9", "10",  
"11", "12"))
```

### Data availability on Italian poverty:

[www.istat.it/it/benessere-e-sostenibilit%C3%A0/obiettivi-di-sviluppo-sostenibile/gli-indicatori-istat](http://www.istat.it/it/benessere-e-sostenibilit%C3%A0/obiettivi-di-sviluppo-sostenibile/gli-indicatori-istat)

The open-source R package: [www.jf-durand-pls.com](http://www.jf-durand-pls.com)

- [Short guide of the R function Bsplines](#)

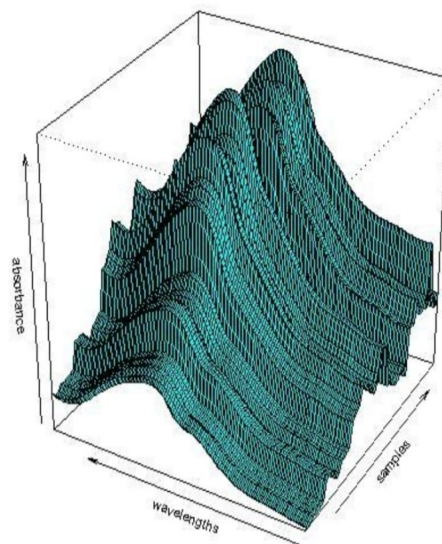
Jean-François Durand

## Boosted Partial Least-Squares regression

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- Durand, JF., Lombardo R., Camminatiello, I., 2025. Identity spline variations in boosted Partial Least-Squares: a study on poverty. *Statistical Methods & Applications*, 34, 1077–1093., (8)

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