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):

  $\boldsymbol{x}$: a sample from the uniform distribution,

  $\boldsymbol{y}$: 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,

    $\longrightarrow$ online local or glolal changes in the observations.
  - Available in any regression method,

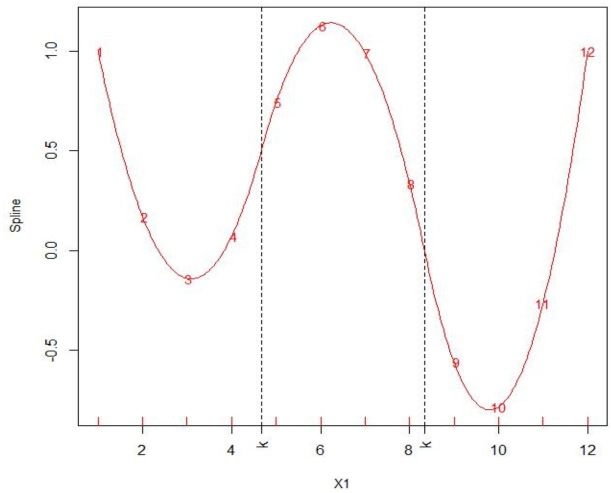
    $\longrightarrow$ here, in Boosted Partial Least-Squares models,

    $\longrightarrow$ to alleviate poverty in the Italian social context.

Contents

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 τ_j whose locations (if any) inside $]a,b[$ and their number K, joined to the degree, are the tuning parameters.

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

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

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

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

2. Splines in bivariate regression

Data: $\{\boldsymbol{x}, \boldsymbol{y}\}$, 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 λ on k-finite differences of adjacent β coefficients**:

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

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

$$\boldsymbol{H} = \boldsymbol{B}(\boldsymbol{B}'\boldsymbol{B} + \lambda\boldsymbol{D}_k'\boldsymbol{D}_k)^{-1}\boldsymbol{B}'$$
$$\hat{\boldsymbol{y}} = \boldsymbol{H}\boldsymbol{y}.$$

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

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

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

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

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

2.2 Interpolation, smoothing and modeling

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

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

- $\boldsymbol{\lambda}$**>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**

$$\boldsymbol{K = n - m \Longrightarrow var(Residuals) = 0}$$

  Drawback: $d > 1$ erratic oscillations.

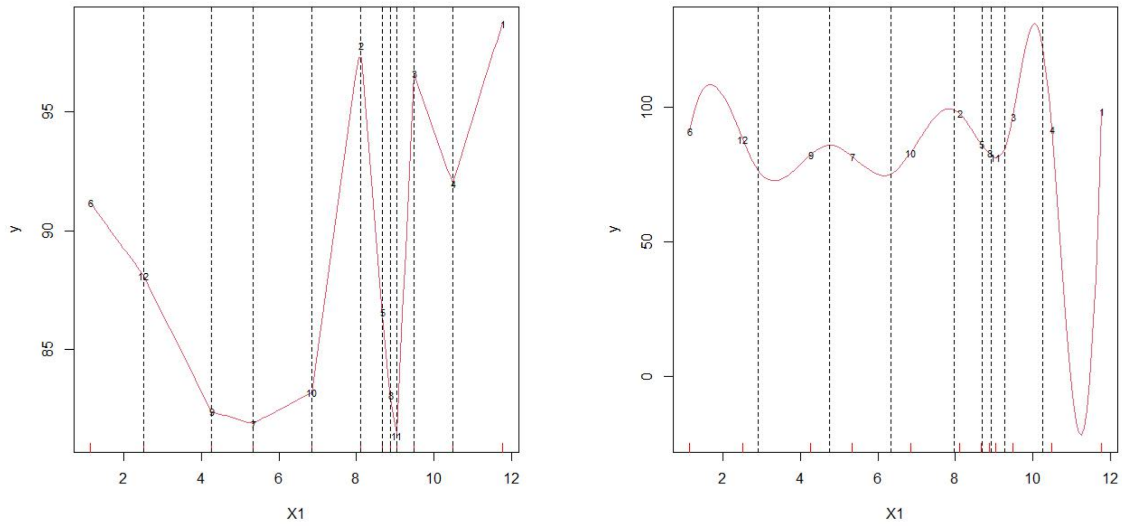
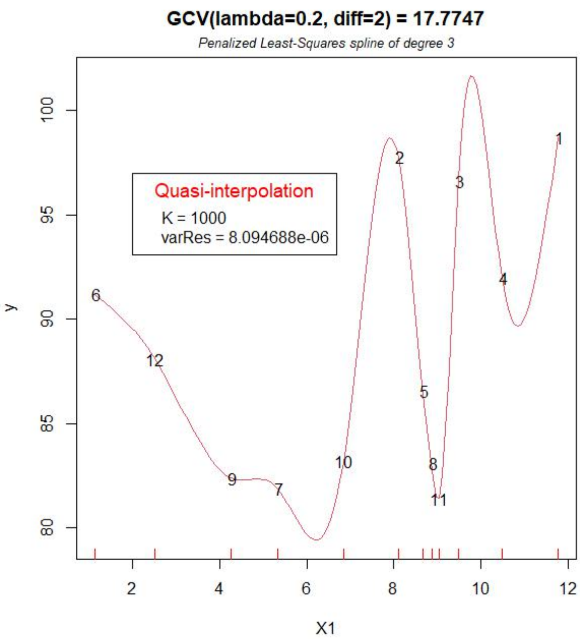


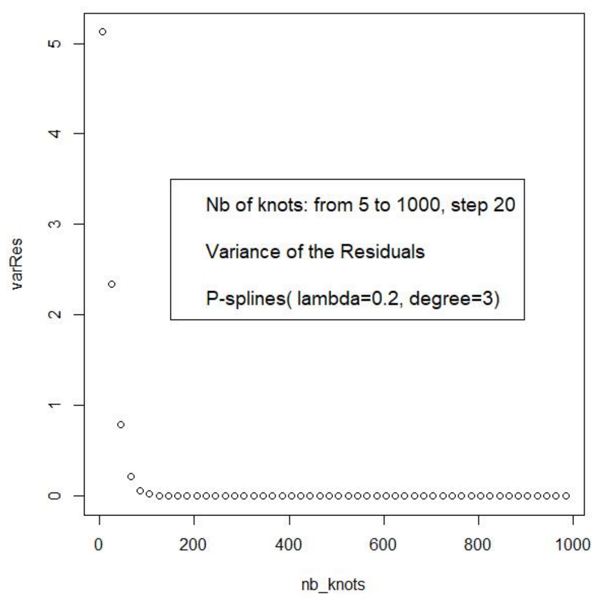
Figure 1: Exact LSS interpolation with knots at quantiles, d=1, K=10 and d=3, K=8.

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

  λ constrains the local curvature and $\lim_{K \to \infty} var(Residuals) = 0$.

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

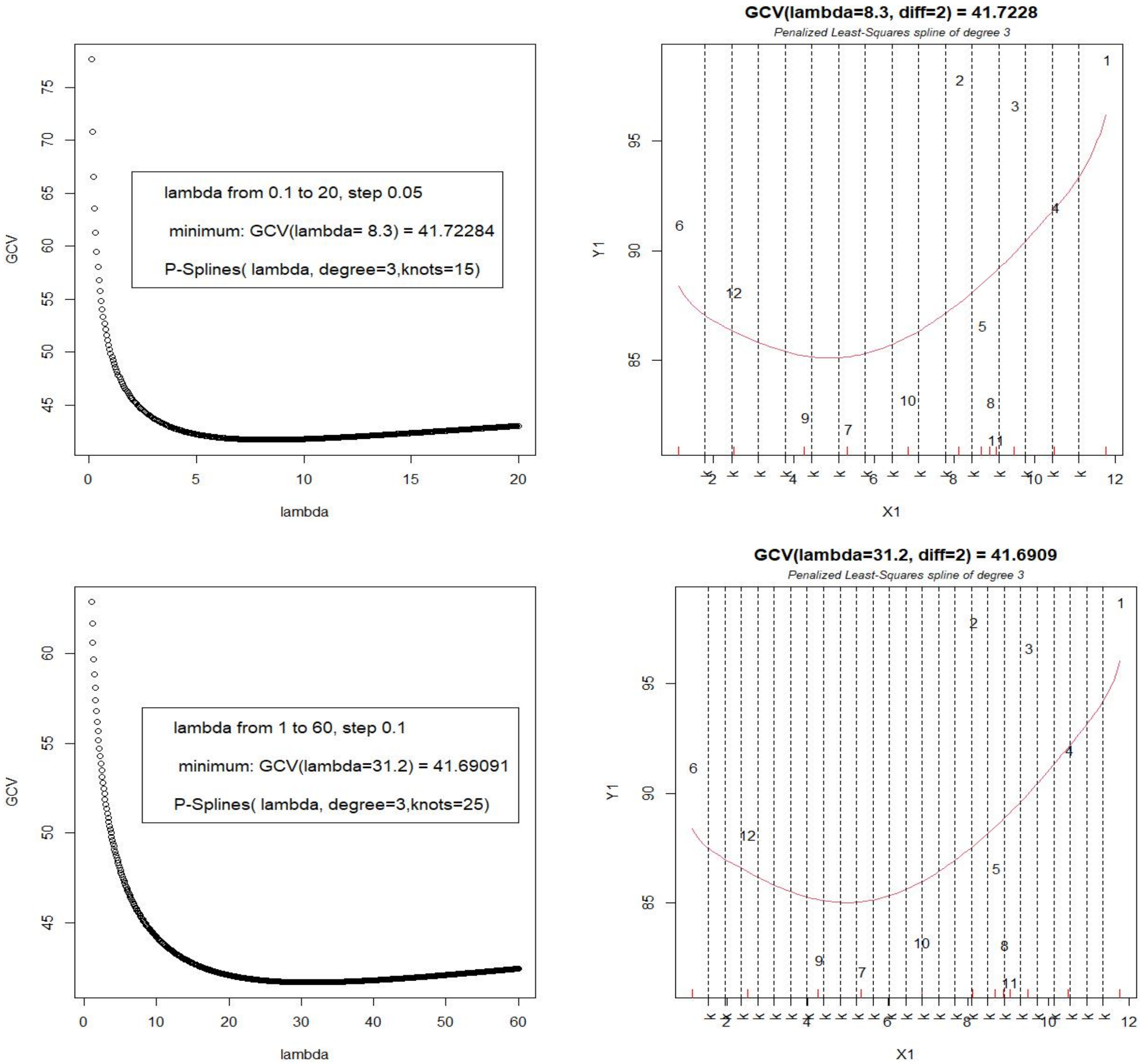




Adaptive-smoothing/Modeling-smoothing: P-splines/LSS

P-splines for λ-adaptive smoothing

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



respectively reveal the best λ values 8.3 and 31.2

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

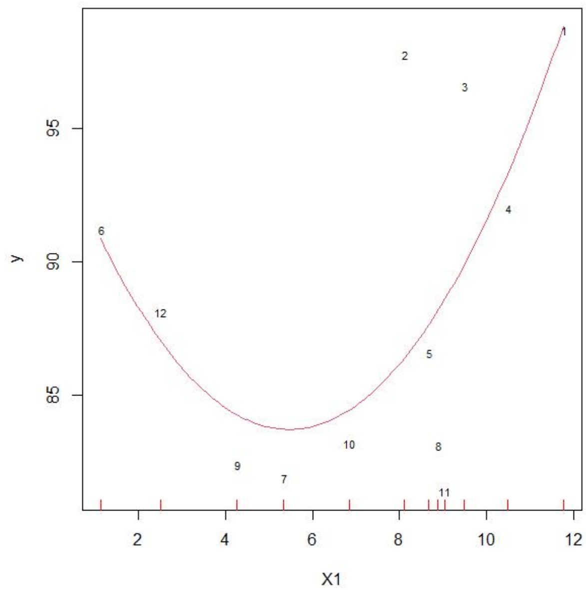
$$GCV(K = 25, \lambda = 31.2) = 41.6909$$

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,

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



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 ($\lambda > 0$):

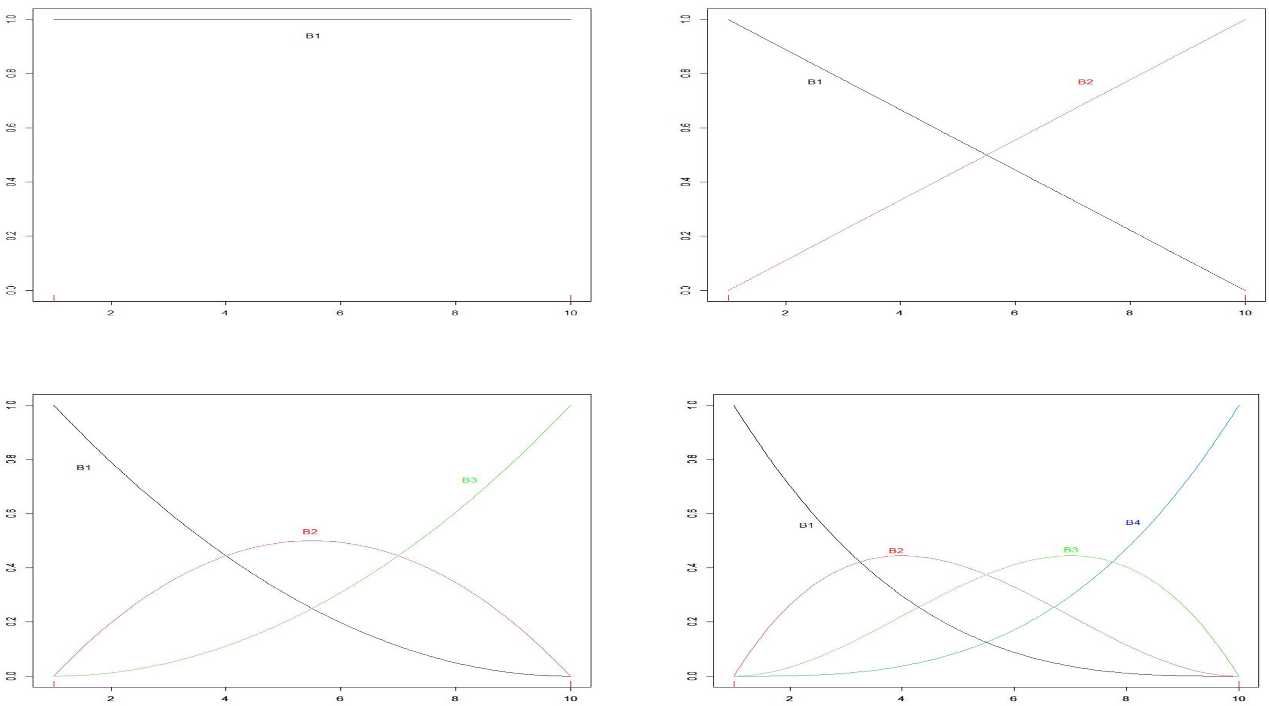
- A robust adaptive smoothing tool to deal with the overfitting issue,
- Non-erratic quasi-interpolation: very large number of knots.

LSS:

- Non-robust: two identical x-observations make $\boldsymbol{B}'\boldsymbol{B}$ 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:

$d=1$: 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 $(1, x)$,

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 $(1, x, x^2)$,

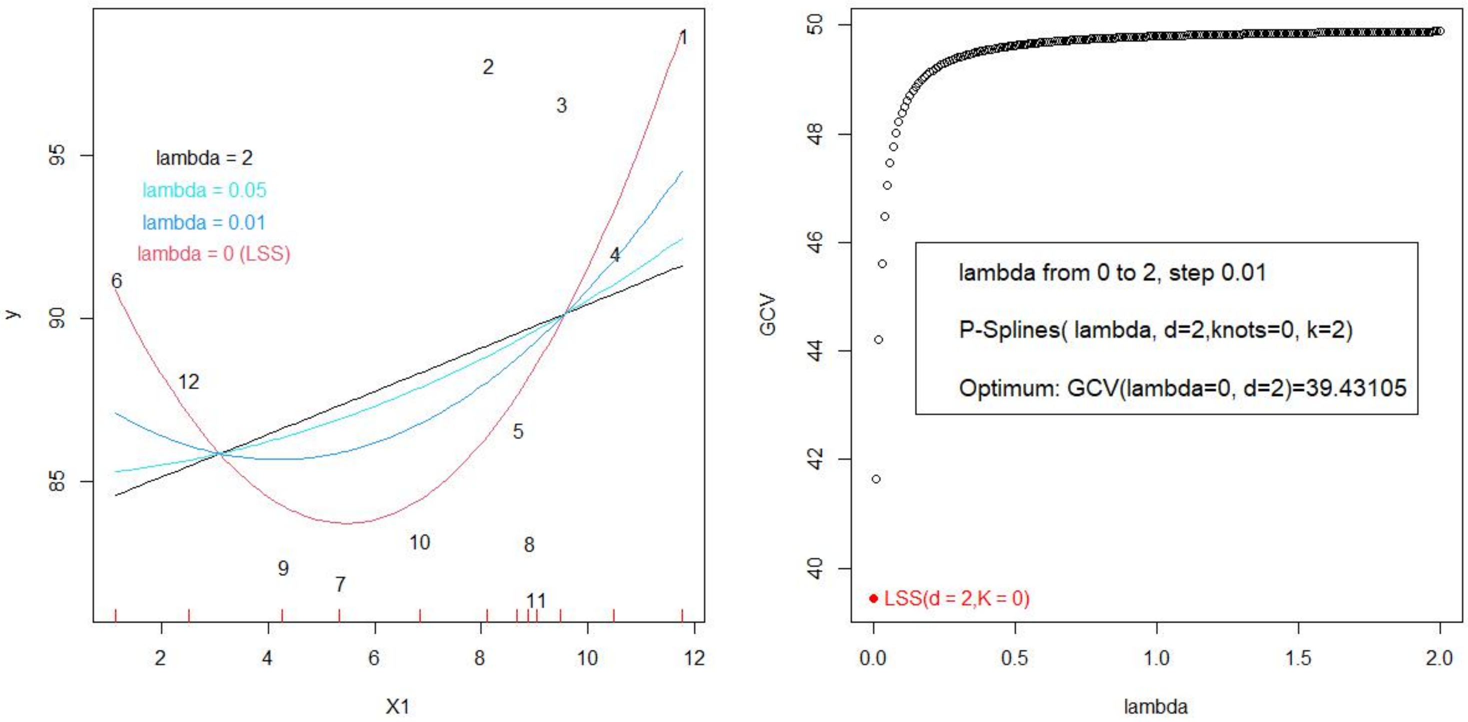
$$\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \frac{1}{(b-a)^2} \begin{bmatrix} b^2 & -2ab & a^2 \\ -2b & 2(a+b) & -2a \\ 1 & -2 & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix}.$$

– P-splines and polynomials:

- $\lambda \longrightarrow +\infty$, 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 $\rightarrow$ degree 1 continuum by more and more constraining the convexity:



- **P1**: Local support

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

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

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

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 τ_j is the number of knots that merge at the same point.

Smoothness at τ_j: C^{d-m_j}:

d	m_j	smoothness at τ_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 $\boldsymbol{\beta}_{\text{nodal}}$ 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 $\boldsymbol{\beta}_{\text{nodal}}$ such that

$$s(x, \boldsymbol{\beta}_{\text{nodal}}) = x$$

are defined by the average of d successive knots.

$$\text{for } j \in 1, ..., m + K, \qquad [\boldsymbol{\beta}_{\text{nodal}}]_j = \frac{1}{d} \sum_{k=1}^{d} \tau_{j+k}.$$

4.2 Identity spline variations. Definition and practice

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

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

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

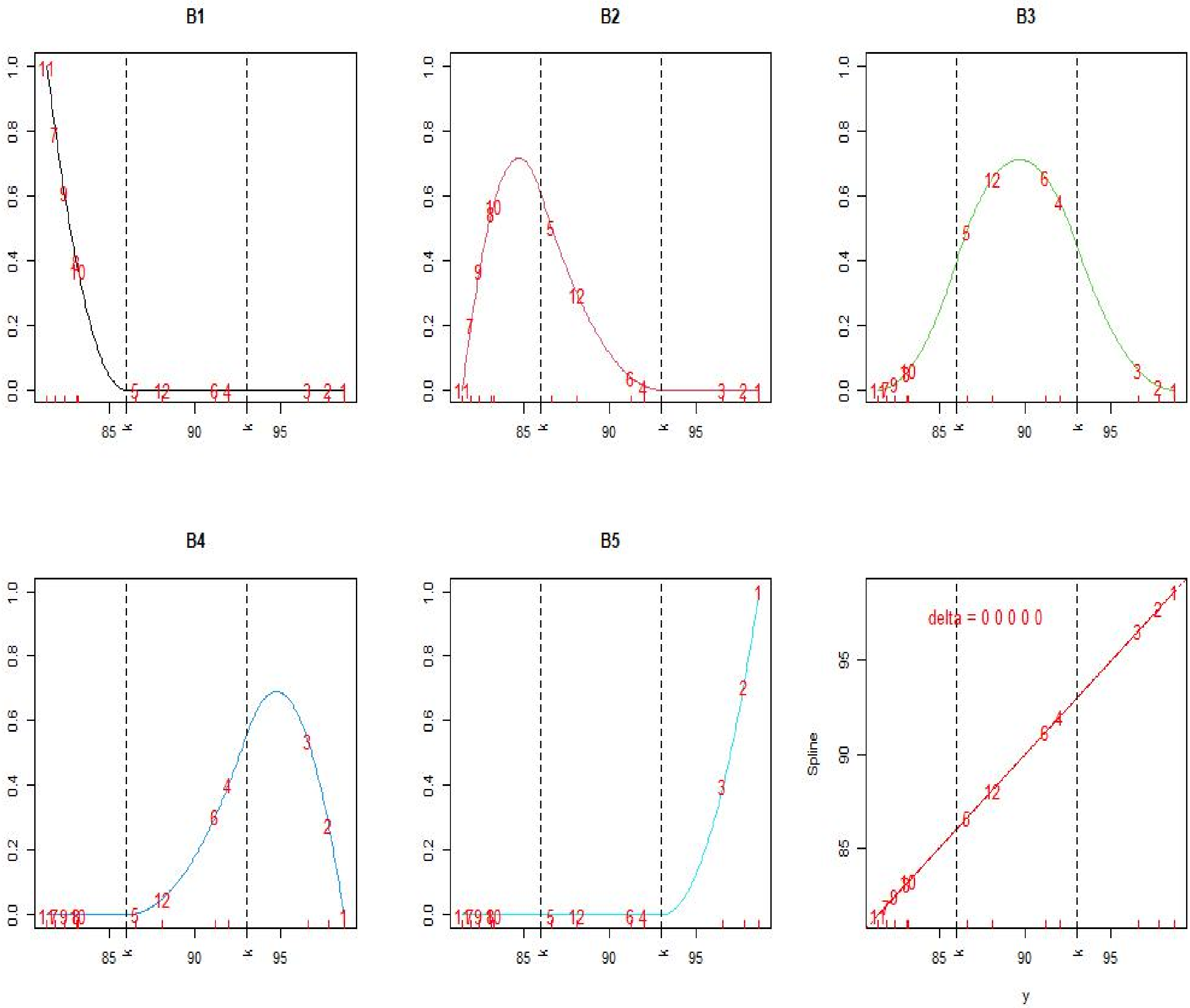


Figure 2: B-splines ($d = 2$, two knots) applied on the cornell data and the spline identity (delta=0).

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

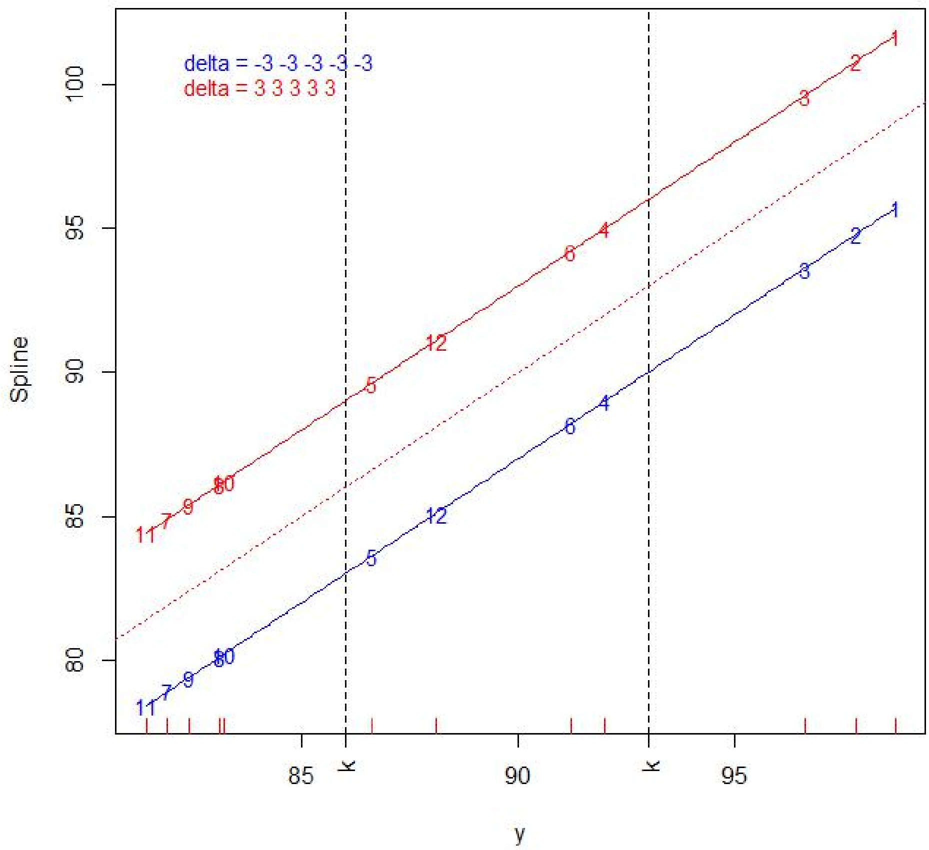


Figure 3: Reversiblility, $\delta = c$, $\delta = -c$, whatever degrees and knots, here $d = 2$, $K = 2$: .

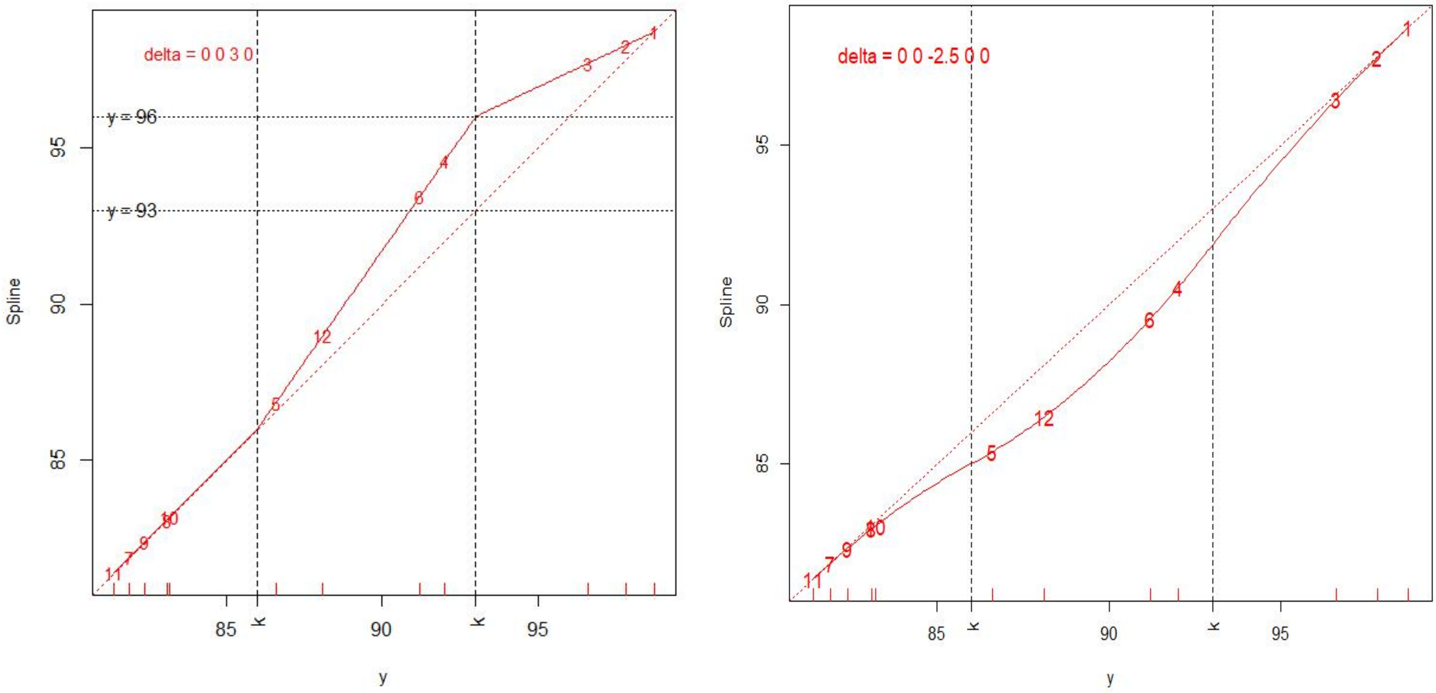


Figure 4: Degree 1 and 2, the identity spline (red dotted line), knots at $86, 93$.

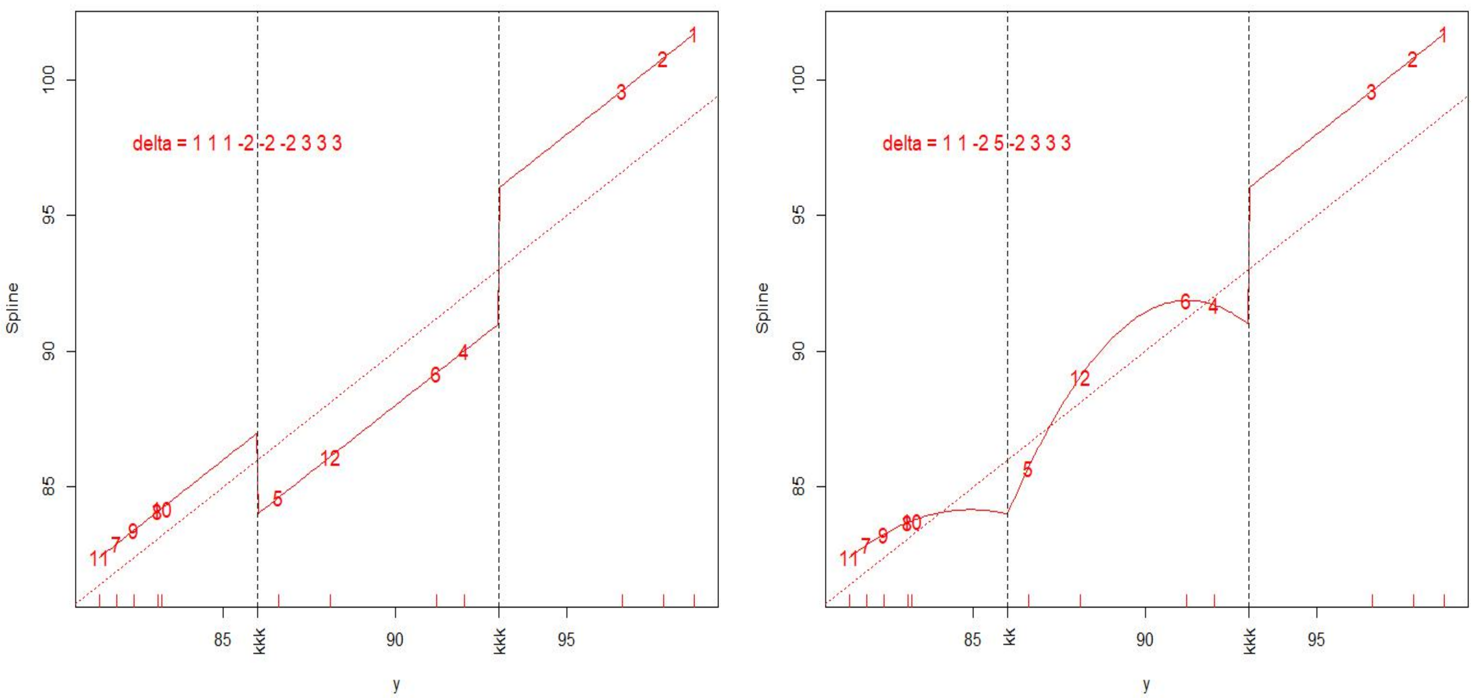


Figure 5: Degree 2 variations with multiple knots. Multiplicity is indicated by overturned k's in x-axis labels.

5. Boosted Partial least-Squares regression

- $\{X = \{x_1, ..., x_p\}, y\}$ standardized variables, n observations.
- A set of B-splines families $B = \{B_1, ..., B_p\}$ associated to X.
- $y(\boldsymbol{\delta})$ 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),

$$\boldsymbol{PLSS(X, y) = PLS(B, y)}.$$

- 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 $t_1, ..., t_A$,

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

In PLSS, the generic component t_i can be expressed as

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

Full dimensioned BPLS: $\boldsymbol{A}=\boldsymbol{r}$, 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

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

- 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 $(\boldsymbol{x}_j, \boldsymbol{y})$ 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 $\{(\boldsymbol{x}_j, \boldsymbol{y})\}_{j=1}^{p}$ scatter plots provides informations to tailor the LSS$(\boldsymbol{x}_j, \boldsymbol{y})$-modeling to the $\boldsymbol{p}$ variables** (GCV$_j$ 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: 20×28 matrix of 28 predictors observed on the 20 regions.

- y_0: the observed Poverty:

$$\text{PLS}_0\text{= PLS}(X, y_0), \quad \text{PLSS}_0\text{= PLSS}(X, y_0).$$

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

$$\text{PLS}_1\text{= PLS}(X, y_1), \quad \text{PLSS}_1\text{= PLSS}(X, y_1).$$

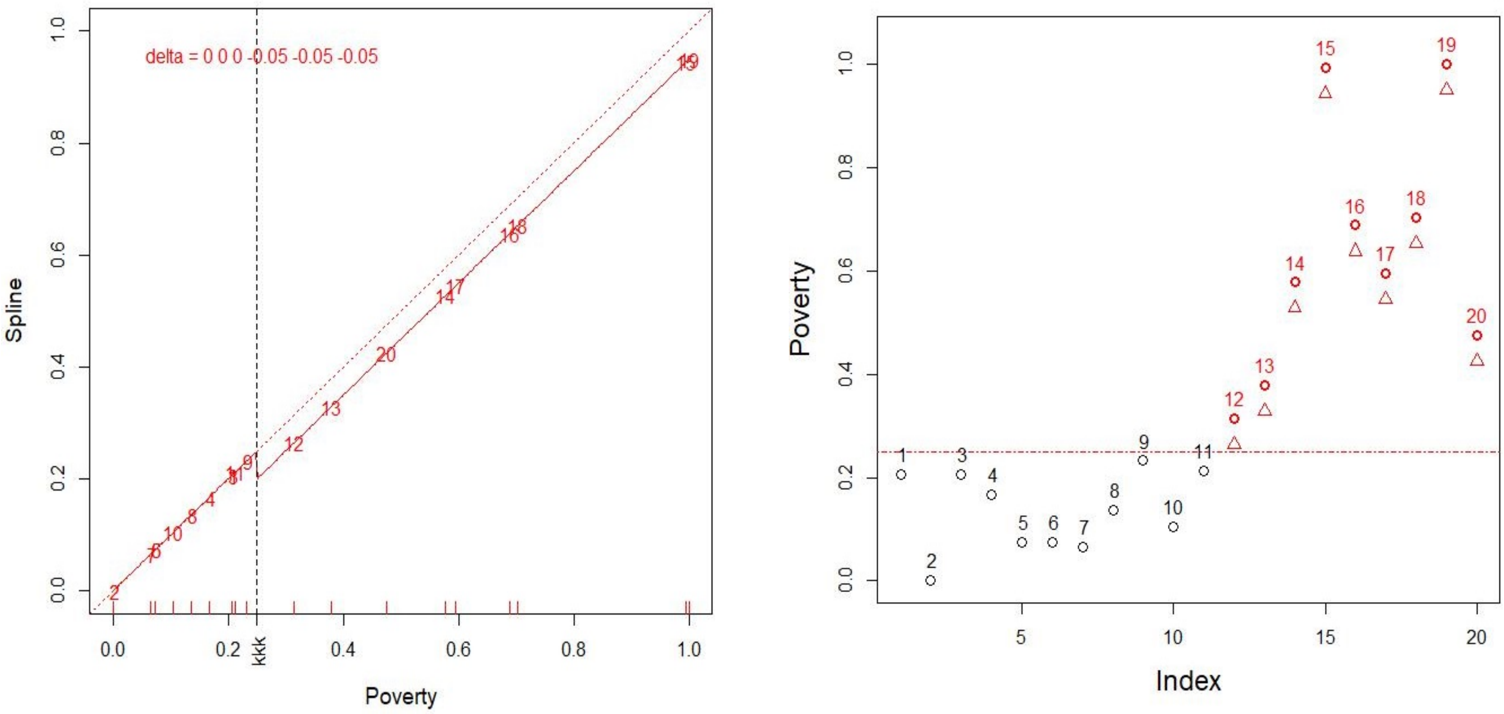


Figure 6: Degree 2, a knot of multiplicity 3 located at 0.25, the poverty average. A Poverty constant delta shift of -0.05 on the 9 most impoverished regions (in red on the left plot).

	PLS$_0$	**PLSS$_0$**	**PLS$_1$**	**PLSS$_1$**
A	4	2	2	2
PRESS	0.057	0.059	0.071	0.070

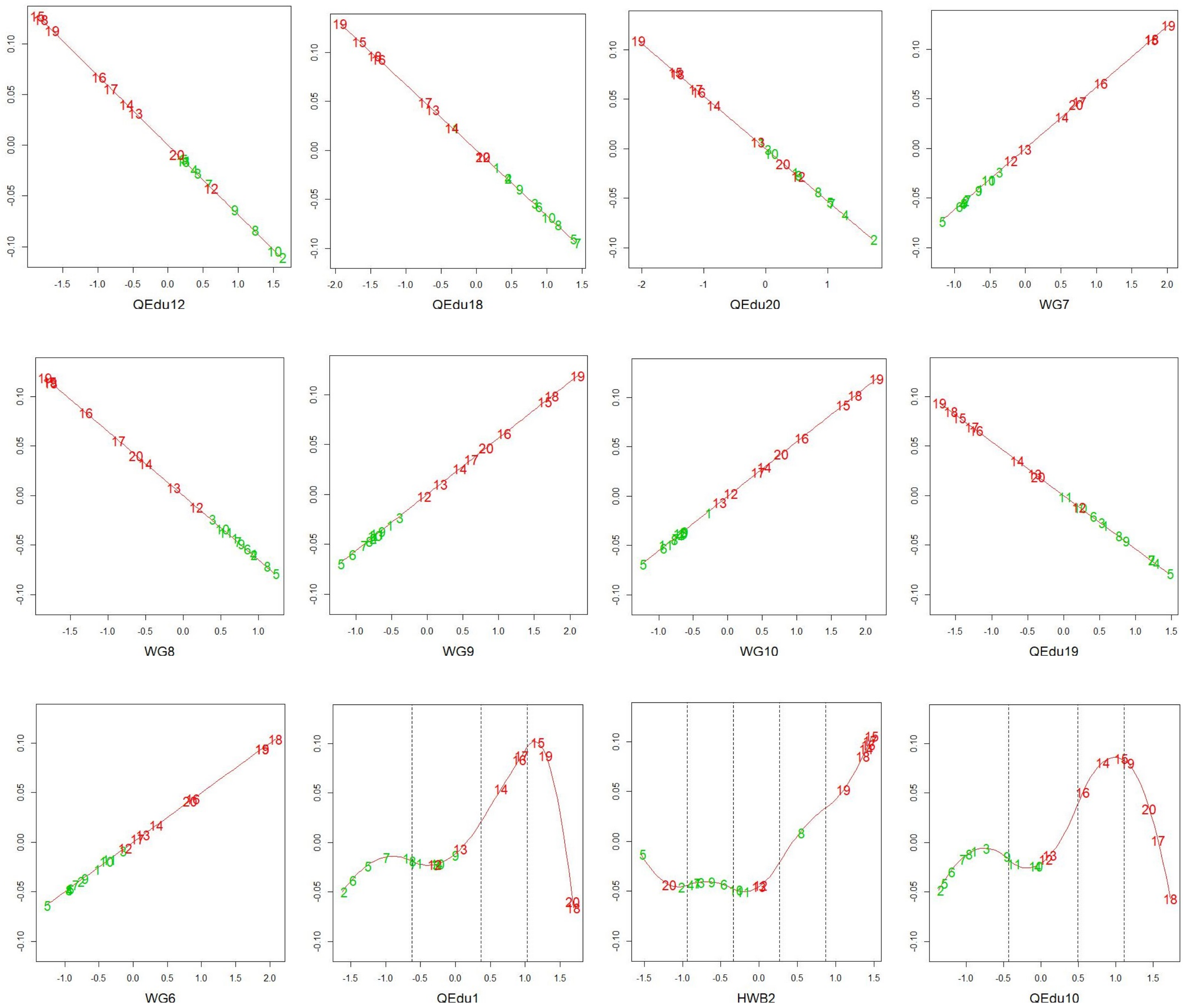


Figure 7: The storyboarded Poverty estimated by PLSS$_1$. The 12 most influential predictors are decreasingly ordered from left to right and up to down according to the range of the coordinate functions.

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.

PLS$_0$	beta	**PLS$_1$**	beta	**PLSS$_0$**	range	**PLSS$_1$**	range	degree	knots
HWB2	0.196	QEdu12	-0.136	QEdu12	0.232	QEdu12	0.238	1	0
HWB3	0.180	HWB2	0.108	QEdu18	0.220	QEdu18	0.224	1	0
HWB5	-0.175	QEdu20	-0.107	WG8	0.196	QEdu20	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 $PLSS_1$ 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 :

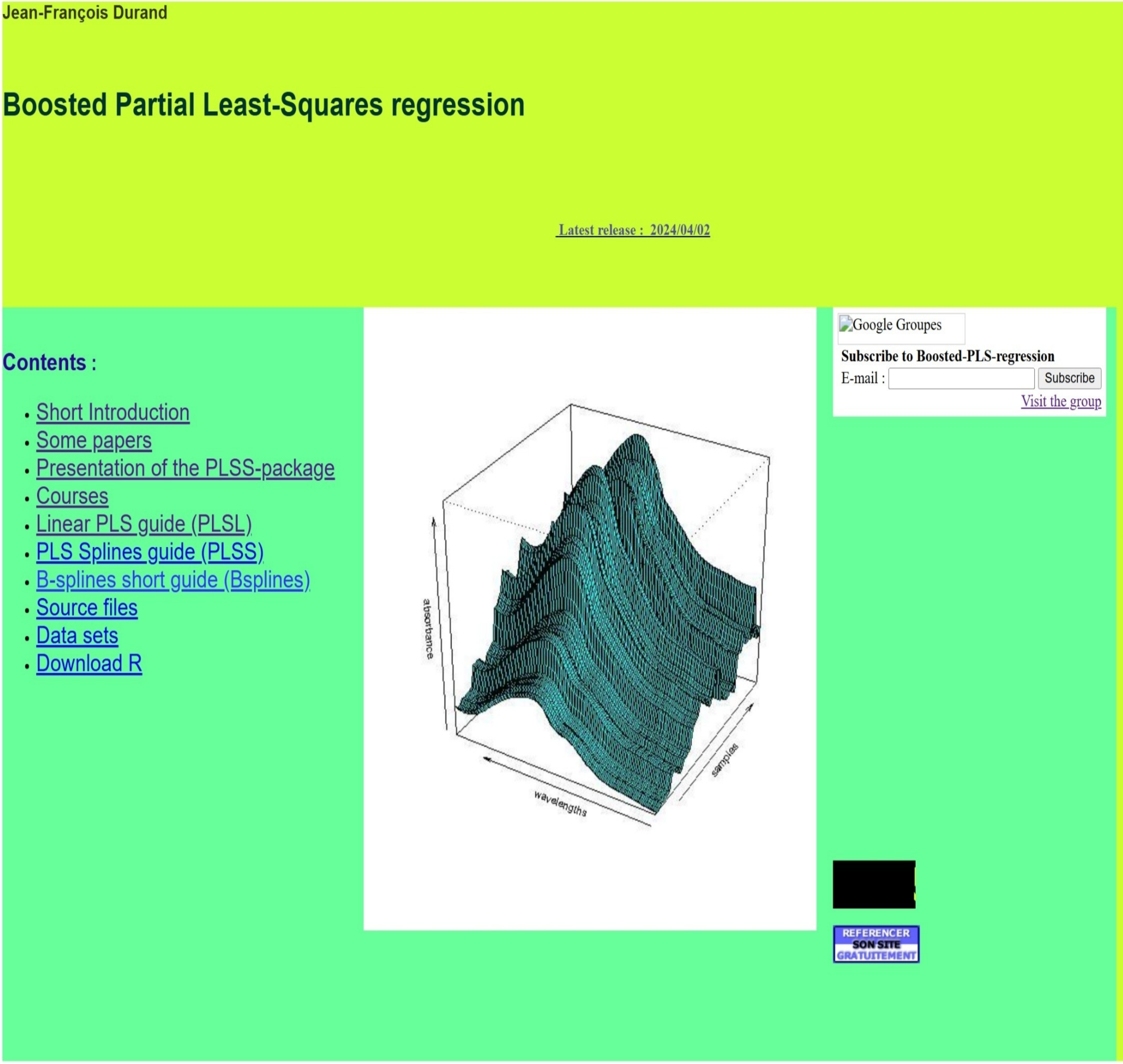
structure(list(xrunif = c(11.7620010608807, 8.09413110627793, 9.4720985062886, 10.4787393852603, 8.65695987828076, 1.12100960616954, 5.3243533782661, 8.86439893278293, 4.26028580009006, 6.8379231570 9.04589922633022, 2.50727575621568), ycornell = c(98.7, 97.8, 96.6, 92, 86.6, 91.2, 81.9, 83.1, 82.4, 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

The open-source R package: www.jf-durand-pls.com

• Short guide of the R function Bsplines



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