Linear algebra of HP-splines

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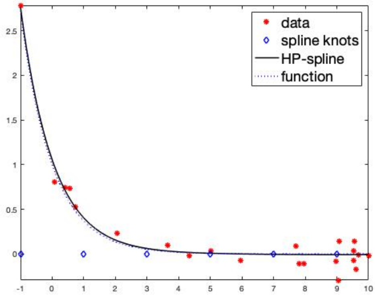
Hyperbolic-polynomial Penalized Splines

Given a set of (noisy) data $(x_i, y_i)_{i=1,\dots,m}$, recently we defined [1] a **regression spline** to approximate **data with exponential trend**



Hyperbolic-Polynomial with segments in the 4-dimensional space

$$\mathbb{E}_{4,\alpha} := \mathrm{span}\{e^{\alpha x},\ x\,e^{\alpha x},\ e^{-\alpha x},\ x\,e^{-\alpha x}\}, \quad \alpha \in \mathbb{R}.$$

[1] *R. C.*, C. Conti, *Penalized Hyperbolic-Polynomial Splines*, Applied Mathematics Letters (2021)

Hyperbolic-polynomial Penalized Splines

Definition

Given a set of (noisy) data $(x_i, y_i)_{i=1,\dots,m}$, and a base of n HB-splines $\{B_j\}_{j=0}^{n+1}$, defined on the uniform set of knots $\{\xi_1, \dots, \xi_n\}$, the coefficients of the **HP-spline** $s_{\alpha,\lambda}(x) = \sum_{j=0}^{n+1} a_j B_j(x_i)$ solve the penalized l.s. problem:

$$\min_{a_0,\dots,a_{n+1}} \sum_{i=1}^{m} \left(y_i - \sum_{j=0}^{n+1} a_j B_j(x_i) \right)^2 + \lambda \sum_{j=0}^{n+1} \left((\Delta_2^{h,\alpha} \mathbf{a})_j \right)^2$$

with the penalty term defined by the difference operator on the coefficients:

$$(\Delta_2^{h,\alpha} \mathbf{a})_j = a_{j+1} - 2e^{-\alpha h} a_j + e^{-2\alpha h} a_{j-1}$$

HP-splines reproduce exponential spaces and **conserve exponential moments** [2]

[2] *R.C.*, C. Conti, *Reproduction Capabilities of Penalized Hyperbolic-polynomial Splines*, arXiv:2202.06678.

Hyperbolic-polynomial Penalized Splines

A study of **the sensitivity with respect to perturbation on the data** is still missing.

Outline:

- Provide a perturbation bound for HP-splines
- Give a criterion to connect this bound to the model parameters in order to better capture the data trend.

HP-splines: a linear algebra approach

HP-splines as a Tikhonov regularization problem in general form:

$$\min_{a\in\mathbb{R}^{n+2}} \|\mathbf{B}_{h\alpha}\mathbf{a}-\mathbf{y}\|_2^2+\lambda^2\|\mathbf{D}_{h\alpha}\mathbf{a}\|_2^2$$

The minimization problem is equivalent to solve the linear system

$$\left(\mathbf{B}_{h\alpha}^T\mathbf{B}_{h\alpha}+\lambda^2(\mathbf{D}_{h\alpha})^T\mathbf{D}_{h\alpha}\right)\mathbf{a}=\mathbf{B}_{h\alpha}^T\mathbf{y},$$

- $\mathbf{y}=(y_1,\ldots,y_m)^T\in\mathbb{R}^m$
- $\mathbf{D}_{h\alpha}\in\mathbb{R}^{n\times(n+2)}$, is the 'difference' matrix:

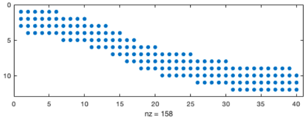
$$\mathbf{D}_{h\alpha}=\begin{bmatrix} 1 & -2e^{-\alpha h} & e^{-2\alpha h} & 0 & \cdots & 0\\ 0 & 1 & -2e^{-\alpha h} & e^{-2\alpha h} & \cdots & 0\\ \vdots & \ddots & \ddots & \ddots & \cdots & \vdots\\ \vdots & \vdots & \vdots & 1 & -2e^{-\alpha h} & e^{-2\alpha h}\end{bmatrix},$$

three-banded, with exponential terms depending on α and h;

HP-splines: a linear algebra approach

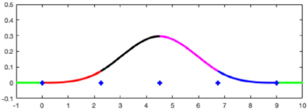
$\mathbf{B}_{h\alpha} \in \mathbb{R}^{m\times(n+2)}$, is the 'collocation' matrix with elements $\mathbf{B}_{h\alpha} := (B_j^{\alpha}(x_i))_{i=1,\dots,m}^{j=1,\dots,n+2}$.

- $\mathbf{B}_{h\alpha}^T$ band structure is inherited by the B-splines locality and depends on the B-splines evaluations at the data x_i;



each HB-spline is:

- with a bell-shaped graph;
- compactly supported, on 5 uniform knots;
- C^2-regular, and with segments in $\mathbb{E}_{4,\alpha}$;



HP-splines: a linear algebra approach

Based on a classical result (see [Theorem 5.1.1, Hansen (1998)]) we define:

Theorem (**Condition number for HP-splines**)

Let $\tilde{\mathbf{a}}_{\alpha,\lambda}$ *be the solution of the perturbed problem*

$$\min_{a} \ \|\tilde{\mathbf{B}}_{h\alpha}\mathbf{a} - \tilde{\mathbf{y}}\|_2^2 + \lambda^2\|\tilde{\mathbf{D}}_{h\alpha}\mathbf{a}\|_2^2.$$

Set $\mathbf{e} = \mathbf{y} - \tilde{\mathbf{y}}$, $\epsilon = \|\mathbf{B}_{h\alpha} - \tilde{\mathbf{B}}_{h\alpha}\|_2/\|\mathbf{B}_{h\alpha}\|_2$, $\mathbf{y}_{\alpha,\lambda} = \mathbf{B}_{h\alpha}\mathbf{a}_{\alpha,\lambda}$, $\mathbf{r}_{\alpha,\lambda} = \mathbf{y} - \mathbf{y}_{\alpha,\lambda}$, $\kappa_{\alpha,\lambda} = \|\mathbf{B}_{h\alpha}\|_2\|\mathbf{X}\|_2/\lambda$, *where* $\mathbf{X}$ *is from the GSVD of* $(\mathbf{B}_{h\alpha}, \mathbf{D}_{h\alpha})$, *then*

$$\frac{\|\mathbf{a}_{\alpha,\lambda} - \tilde{\mathbf{a}}_{\alpha,\lambda}\|_2}{\|\mathbf{a}_{\alpha,\lambda}\|_2} \leq \frac{\kappa_{\alpha,\lambda}}{1 - \epsilon\kappa_{\alpha,\lambda}}\left((1 + cond(\mathbf{X}))\epsilon + \frac{\|\mathbf{e}\|_2}{\|\mathbf{y}_{\alpha,\lambda}\|_2} + \epsilon\kappa_{\alpha,\lambda}\frac{\|\mathbf{r}_{\alpha,\lambda}\|_2}{\|\mathbf{y}_{\alpha,\lambda}\|_2}\right), \quad 0 < \lambda \leq 1$$

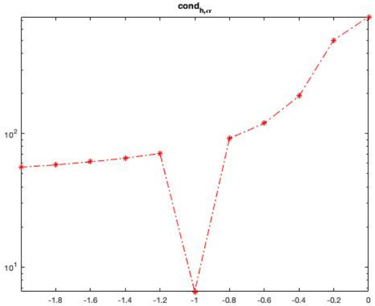
Moreover, if $\epsilon = 0$ *and* $\lambda < 1/\sqrt{2}$, *the tighter bound holds:*

$$\frac{\|\mathbf{a}_{\alpha,\lambda} - \tilde{\mathbf{a}}_{\alpha,\lambda}\|_2}{\|\mathbf{a}_{\alpha,\lambda}\|_2} \leq \frac{\kappa_{\alpha,\lambda}}{2(1-\lambda^2)^{1/2}}\frac{\|\mathbf{e}\|_2}{\|\mathbf{y}_{\alpha,\lambda}\|_2}.$$

Numerical example: condition number as α varies

Set $f(x) = e^{-x}$:

1. $[a, b] = [0, 10]$,
2. 77 data points (x_i, y_i), $x_i \in [a, b]$, $y_i = f(x_i)$;
3. $n = 21$ knots distributed in $[a, b]$ with $h = 0.5$;
4. $\alpha \in [-2, 0)$



The condition number $cond_{\alpha,\lambda} := \frac{\kappa_{\alpha,\lambda}}{1-\epsilon\kappa_{\alpha,\lambda}}$ strongly depends on the α values.

Numerical example: condition number as α varies

Set $f(x) = e^{-x}$:

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3. $n = 21$ knots distributed in $[a, b]$ with $h = 0.5$;
4. $\alpha \in [-2, 0)$

α	λ	$cond_{\alpha,\lambda}$	$\epsilon_{\alpha,\lambda}$
-2.0000e+00	1.0428e-01	5.6008e+01	6.2447e-03
-1.8000e+00	9.0319e-02	5.8300e+01	3.8669e-03
-1.6000e+00	7.6168e-02	6.1390e+01	2.1007e-03
-1.4000e+00	6.2135e-02	6.5457e+01	9.0026e-04
-1.2000e+00	4.8566e-02	7.0891e+01	2.1672e-04
-1.0000e+00	**8.5980e-01**	**6.5602e+00**	**1.9259e-15**
-8.0000e-01	2.4343e-02	9.1996e+01	2.0032e-04
-6.0000e-01	1.4518e-02	1.1917e+02	7.6932e-04
-4.0000e-01	6.8365e-03	1.9067e+02	1.6608e-03
-2.0000e-01	1.8116e-03	5.0035e+02	2.8320e-03
6.9389e-14	1.8453e-03	7.4674e+02	1.1095e+00

The relative error on the solution $s_{\alpha,\lambda}$ is computed at uniformly distributed points:

$$\epsilon_{\alpha,\lambda} = \frac{\|s_{\alpha,\lambda}(\mathbf{v}) - f(\mathbf{v})\|}{\|f(\mathbf{v})\|}, \quad \mathbf{v} = (v_i)_{i=1}^{\ell}, \quad \ell = 1000$$

Free parameters and data-driven strategy

- The knots distance h is related to the **discretization error** of the penalty term $\Delta_2^{h,\alpha}$.
- The frequency α defines the spline space

$$\mathbb{E}_{4,\alpha} := \mathrm{span}\{e^{\alpha x},\ x\,e^{\alpha x},\ e^{-\alpha x},\ x\,e^{-\alpha x}\}, \quad \alpha \in \mathbb{R},$$

  and behaves like a **shape parameter** and gives information on the data-trend;
- The regularization parameter λ affects **the smoothing effects of the HP-spline**;

Idea

To analyze the impact of α to control the perturbations on the solution:

– Make explicit α in $cond_{\alpha,\lambda}$;

– Propose a criterion to select *a good* α to capture the trend of the assigned data.

An algorithm to tune α

set α_0 $\leftarrow$ (1) Fixed an initial guess
$it = 1$, $ind = 1$, $step = 0$, $cond_{\alpha_0,\lambda_0} = 0$, $maxit = 15$
$\alpha^* = \alpha_0 - 0.5$
while $step < 4$ and $it <= maxit$ **do** $\leftarrow$ (2) choose $\alpha = \arg\min_{\alpha^*} cond_{\alpha^*,\lambda^*}$
  compute GSVD of $(\mathbf{B}_{h\alpha}, \mathbf{D}_{h\alpha})$
  compute λ^* by L-curve
  if $\lambda^* > 0$ and $\lambda^* <= 1$ **then**
    compute $cond_{\alpha^*,\lambda^*}(ind)$
  end if
  if $ind >= 2$ and $cond_{\alpha^*,\lambda^*}(ind) > cond_{\alpha^*,\lambda^*}(ind-1)$ **then**
    $step = step + 1$
  end if
  $\alpha^* = \alpha^* + 0.15$
  $ind = ind + 1$
  $it = it + 1$
end while

(1) $\alpha_0 = c_3$ is defined by nonlinear least-squares regression of the data using the parametric function $g(\mathbf{c}, x) = c_1 e^{c_3 x} + c_2 e^{-c_3 x}$

An algorithm to tune α

(2) choose $\alpha = \arg\min_{\alpha^*} cond_{\alpha^*,\lambda^*}$

Idea

Study $cond_{\alpha,\lambda}$ w.r.t. α.

Make explicit the dependence of $\kappa_{\alpha,\lambda} = \|\mathbf{B}_{h\alpha}\|_2 \|\mathbf{X}\|_2/\lambda$, w.r.t. α.

As for $\|\mathbf{B}_{h\alpha}\|_2$

- Each column contains the evaluations of HB-splines $\{B_0, \ldots, B_{n+1}\}$ at $\{x_i\}_{i=1,\ldots,m}$.
- HB-splines have been defined[3] in terms of Bernstein(-like) local bases
- An explicit expression in terms of α for the $\{B_0, \ldots, B_{n+1}\}$ **is needed**.

[3] *R. C.*, C. Conti, S. Cuomo, Smoothing exponential-polynomial splines for multiexponential decay data, DRNA (2019)

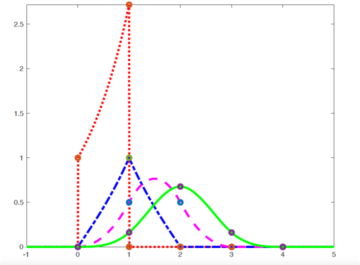
Following [Unser,2005] we compute the HB-splines through convolution:

From the HB-spline of *order 1* $B^1_\alpha(x) = e^{\alpha\, x}\chi_{[0,1]}(x)$ supported in $[0,1]$,

- the cardinal HB-spline of *order 4* in $[0,4]$ is obtained as

$$B^1_{\boldsymbol{\alpha}} = \left(B^1_\alpha * B^1_\alpha * B^1_{-\alpha} * B^1_{-\alpha}\right) \quad \text{with} \quad \boldsymbol{\alpha} = (\alpha, \alpha, -\alpha, -\alpha).$$

- all the HB-splines supported in $[k, k+4]$ are obtained by translation as $B^1_{\boldsymbol{\alpha}}(\cdot - k)$.



Cardinal HB-splines of order 4 (green) is obtained by convolution of 4 HB-splines of order 1 (red)

When $h \neq 1$, the HB-splines are defined by dilation,

$$B^h_{h\boldsymbol{\alpha}} = B^1_{\boldsymbol{\alpha}}(\frac{\cdot}{h}) = \left(B^1_\alpha * B^1_\alpha * B^1_{-\alpha} * B^1_{-\alpha}\right)(\frac{\cdot}{h}),$$

and then translation.

Proposition

The HB-spline of order 4, with uniformly distributed knots, $t_k = kh$, $k = 0, \ldots, 4$, and with frequencies $\boldsymbol{\alpha} = (\alpha, \alpha, -\alpha, -\alpha)$, $B^h_{h\boldsymbol{\alpha}}$, is piecewise define as

$$\begin{cases} \frac{t}{h} p_\alpha(t) - \frac{1}{h\alpha} m_\alpha(t) & t \in (0, h] \\ -\alpha(t-h)p_\alpha(t-2h) - \left(\frac{t-2h}{h}\right) p_\alpha(t) + \frac{2}{h\alpha} m_\alpha(t-2h) + \frac{1}{h\alpha} m_\alpha(t) & t \in (h, 2h] \\ \left(\frac{t-2h}{h}\right) p_\alpha(t-4h) + 2\left(\frac{t-3h}{h}\right) p_\alpha(t-2h) - \frac{1}{h\alpha} m_\alpha(t-4h) - \frac{2}{h\alpha} m_\alpha(t-2h) & t \in (2h, 3h] \\ -(t-4h)p_\alpha(t-4h) + \frac{1}{h\alpha} m_\alpha(t-4h) & t \in (3h, 4h] \end{cases}$$

with $p_\alpha(t) = e^{\alpha t} + e^{-\alpha t}$ and $m_\alpha(t) = e^{\alpha t} - e^{-\alpha t}$.

Sensitivity analysis: a parametric perturbation bound

Lemma

The 1-norm of the collocation matrix $\mathbf{B}_{h\alpha}$*, is bounded by:*

$$\|\mathbf{B}_{h\alpha}\|_2 \leq \sqrt{n+2}\|\mathbf{B}_{h\alpha}\|_1 \leq \sqrt{n+2}\frac{m}{(n+1)}\left(\frac{1}{h\alpha}(e^{\alpha\, 2h} - e^{-\alpha\, 2h}) - \alpha\, h\, 2\right)$$

As for $\|\mathbf{X}\|_2$

- From the GSVD of $(\mathbf{B}_{h\alpha}, \mathbf{D}_{h\alpha})$, it holds [Hansen, 1998]: $\|\mathbf{X}\|_2 \approx \|\mathbf{D}^{\dagger}_{h\alpha}\|_2$;
- $\|\mathbf{D}_{h\alpha}\|_1 = 1 + 2e^{-\alpha\ h} + e^{-2\alpha\ h}$.

We give the *parametric estimate*

$\kappa_{\alpha,\lambda} = \|\mathbf{B}_{h\alpha}\|_2\|\mathbf{X}\|_2/\lambda$ can be approximated as:

$$\kappa_{\alpha,\lambda} \approx \mathcal{F}(\alpha) = \frac{\sqrt{n+2}}{\lambda}\,\frac{m}{(n+1)}\,\frac{\left(\frac{1}{h\alpha}(e^{\alpha\, 2h} - e^{-\alpha\, 2h}) - \alpha\, h\, 2\right)}{(1 + 2e^{-\alpha\ h} + e^{-2\alpha\ h})}$$

Numerical examples

Set $f(x) = e^{-x}$:

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2. 77 data points (x_i, y_i), $x_i \in [a, b]$, $y_i = f(x_i)$;
3. $n = 21$ knots distributed in $[a, b]$ with $h = 0.5$;
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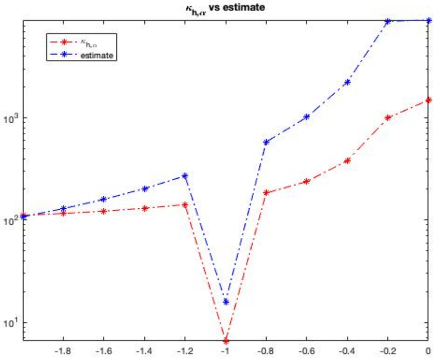
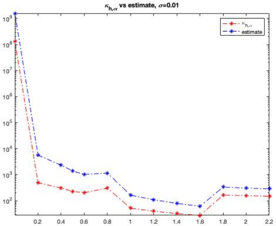
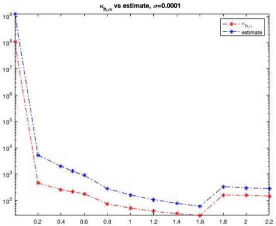


The estimate (blue '*') boundes the $\kappa_{\alpha,\lambda}$ (red '*') for different α values.

Numerical examples

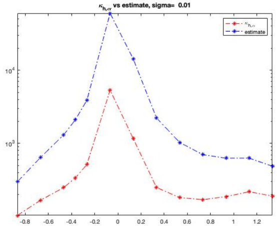


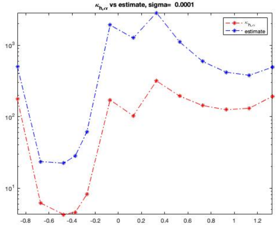


$f(x) = e^{x/2} + e^{-2x}$, $\alpha \in [-0.4, 2.2]$

α	$cond_{\alpha,\lambda}$	$\tilde{cond}_{\alpha,\lambda}$	$\epsilon_{\alpha,\lambda}$, $\sigma = 10^{-2}$
5.0038e-01	1.1358e+02	6.8831e+02	1.0187e-05
6.0038e-01	1.0195e+02	5.1021e+02	1.1043e-05
8.0038e-01	1.5188e+02	5.7731e+02	5.9820e-06
1.0004e+00	2.6125e+01	8.2612e+01	1.6338e-05
1.2004e+00	2.0335e+01	5.6091e+01	1.8108e-05
1.4004e+00	1.7302e+01	4.2666e+01	2.0294e-05
1.6004e+00	1.6587e+01	3.6997e+01	2.3687e-05
1.8004e+00	8.2283e+01	1.6862e+02	1.5545e-05
α	$cond_{\alpha,\lambda}$	$\tilde{cond}_{\alpha,\lambda}$	$\epsilon_{\alpha,\lambda}$, $\sigma = 10^{-4}$
5.0043e-01	1.0663e+02	6.4613e+02	1.0861e-05
6.0043e-01	9.0014e+01	4.5042e+02	1.2283e-05
8.0043e-01	3.7652e+01	1.4311e+02	1.5228e-05
1.0004e+00	2.5968e+01	8.2114e+01	1.6887e-05
1.2004e+00	2.0303e+01	5.5999e+01	1.8969e-05
1.4004e+00	1.7293e+01	4.2642e+01	2.1608e-05
1.6004e+00	1.6586e+01	3.6992e+01	2.5697e-05
1.8004e+00	8.2282e+01	1.6861e+02	1.7297e-05

Numerical examples





$f(x) = 1/\sqrt{1+s^2}$, $\alpha \in [-0.4, 2.2]$			
α	$cond_{\alpha,\lambda}$	$\tilde{cond}_{\alpha,\lambda}$	$\epsilon_{\alpha,\lambda}$, $\sigma = 10^{-2}$
-8.6720e-01	5.2075e+01	1.5002e+02	6.8500e-04
-6.6720e-01	8.3848e+01	3.2215e+02	6.9168e-04
-4.6720e-01	1.2501e+02	6.5704e+02	6.9362e-04
-3.6720e-01	1.6890e+02	1.0517e+03	6.9417e-04
-2.6720e-01	2.5818e+02	1.9474e+03	6.9453e-04
-6.7196e-02	2.6748e+03	2.9998e+04	6.9502e-04
1.3280e-01	5.8018e+02	7.1051e+03	6.9501e-04
3.3280e-01	1.2528e+02	1.1156e+03	6.9519e-04
α	$cond_{\alpha,\lambda}$	$\tilde{cond}_{\alpha,\lambda}$	$\epsilon_{\alpha,\lambda}$, $\sigma = 10^{-4}$
-8.7175e-01	8.7838e+01	2.5148e+02	9.0979e-07
-6.7175e-01	3.9159e+00	1.4942e+01	2.6564e-04
-4.7175e-01	2.9058e+00	1.5159e+01	3.7669e-04
-3.7175e-01	2.7340e+00	1.6888e+01	3.4258e-04
-2.7175e-01	4.2485e+00	3.1739e+01	2.3780e-04
-7.1752e-02	8.5454e+01	9.5436e+02	8.0437e-05
1.2825e-01	5.1304e+01	6.2900e+02	2.1873e-05
3.2825e-01	1.5783e+02	1.4201e+03	2.7648e-06

Conclusions

Main results:

- To derive **a perturbation bound**;
- To give **an estimate of the condition number in terms of some model parameters**.

This technique gives a criterion for a data-driven selection of α, also reducing the computational cost required by repeated GSVDs.

Future aims:

An improvement of the bound: to study $\min_{h,\alpha} \mathcal{F}(h, \alpha)$

- to compute the minimum value;
- to find the correspondence with the optimal α and h.

Thanks for your attention