A linear algebra approach to HP-splines frequency parameter selection

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Abstract

In this work we propose a strategy to select the frequency parameter of hyperpolic-polynomial P-splines, HP-splines for shortness. HP-splines are hyperpolic-polynomial penalized splines where polynomials are replaced by the richer class of exponential-polynomials and a tailored discrete penalty term is used. HP-splines reduce to P-splines when setting the frequency parameter to zero but are more suitable to data with an exponential trend, which are frequently encountered in applications. Yet, they require an effective strategy to select the frequency parameter in addition to the one needed for selecting the smoothing parameter. Here, we propose a strategy that involves a linear algebra approach for Tikhonov regularization problems adapted to HP-splines. As shown in the numerical experiments, our strategy provides an efficient criterion yielding to HP-splines that better capture the trend suggested by the fitted data.

Keywords: Hyperbolic-polynomial splines, Penalized splines, Condition number, P-splines, B-splines and HB-splines

1. Introduction

The use of splines and B-splines for smoothing and data fitting has a very long history, see [1–4], only to mention some examples. *Penalized splines* are well established tools for data regression. Given the data points (x_i, y_i), $i = 1, \dots, m$ and the spline space spanned by a suitable basis $\{b_0 \cdots, b_{n+1}\}$, a *penalized spline* $s(x) = \sum_{j=0}^{n+1} a_j b_j(x)$ is obtained by solving a penalized weighted least square problem

$$\arg \min_{\mathbf{a}\in\mathbb{R}^{n+2}} \sum_{i=1}^{m} w_i \left(y_i - s(x_i)\right)^2 + \lambda^2 R(\mathbf{a}), \quad \mathbf{a} = (a_0, \cdots a_{n+1}), \tag{1}$$

where $w_1, \dots, w_m$ are weights, λ is a *smoothing* or *regularization* parameter and $R(\mathbf{a})$ is a *penalty* term. As well known, an open issue in penalized models is the selection of the regularization parameter since the result is highly dependent on its proper choice that guarantees a fair balance between the *perturbation* error and the *regularization* error. Classical strategies for the smoothing parameter selection are based on the minimization of the mean squared error or, alternatively, on a linear mixed model where the smoothing parameter is interpreted as the *a priori* variance of spline coefficients so that the maximum likelihood theory can be used to determine it as a variance component [5]. Other ways to tune the smoothing parameter are based on generalized cross-validation or on the Akaike information criterion [6], as well as the L-curve approach, originally developed for ridge regression [7]. See [8] and [9] for a comparison between different techniques.

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A special instance of penalized splines are P-splines proposed twenty five years ago by P.H.C. Eilers and B.D. Marx (see [10] and also [6]). P-splines are based on two main ingredients: polynomial B-splines and discrete difference penalties. In the cubic case, the penalty is written in terms of the splines coefficients as

$$R(\mathbf{a}) = \sum_{j=2}^{n+1} \Big((\Delta_2 \mathbf{a})_j \Big)^2, \quad \text{where} \quad (\Delta_2 \mathbf{a})_j = a_j - 2a_{j-1} + a_{j-2}, \quad j = 2, \dots, n+1. \tag{2}$$

Going beyond P-splines, in [11] the authors have proposed HP-splines, the class of penalized splines where the richer space of hyperbolic-polynomial splines replaces the polynomial spline space. They consist of piecewise-defined functions with segments in the four-dimensional parametric space

$$\mathbb{E}_{4,\alpha} := \text{span}\{e^{\alpha x},\ x\, e^{\alpha x},\ e^{-\alpha x},\ x\, e^{-\alpha x}\},\ \alpha \in \mathbb{R}, \tag{3}$$

and reduce to cubic splines for $\alpha = 0$.

The hyperbolic-polynomial splines here defined are just a very special instance of the so called Tchebyceffian splines, introduced and analyzed decades ago by L.L. Schumaker and some coauthors (see [12]) but the specific space in (3) derives from [13], a previous work by the authors, where a smoothing exponential-polynomial spline was defined for multiexponential decay data.

Similarly to the polynomial case, the two main ingredients of HP-splines are: HB-splines, a basis for the space of piecewise hyperbolic-polynomial functions with similar properties than polynomial B-splines, and an α-dependent penalty term.

More in details, if $\{B_0^\alpha(x), \cdots, B_{n+1}^\alpha(x)\}$ are HB-splines depending on the space (or frequency) parameter α, the penalized HP-spline $s(x) = \sum_{j=0}^{n+1} a_j B_j^\alpha(x)$, is defined by solving the penalized least square problem (1) where the penalty is written in terms of the splines coefficients as

$$R(\mathbf{a}) = \sum_{j=2}^{n+1} \Big((\Delta_2^{h,\alpha} \mathbf{a})_j \Big)^2, \quad \text{where} \quad (\Delta_2^{h,\alpha} \mathbf{a})_j = a_j - 2e^{-\alpha h} a_{j-1} + e^{-2\alpha h} a_{j-2}, \quad j = 2, \dots, n+1. \tag{4}$$

Note that, the operator $(\Delta_2 \mathbf{a})_j$ is an annihilation operator for sequences sampled from linear polynomial while $(\Delta_2^{h,\alpha} \mathbf{a})_j$ is an annihilation operator for sequences sampled from functions in the exponential polynomial space $\{e^{-\alpha x}, xe^{-\alpha x}\}$. This fact is important and it is the reason why the HP-spline model reproduces $\{e^{-\alpha x}, xe^{-\alpha x}\}$ as shown in [14].

Due to their nature, HP-splines are more suitable in application where the data show a multi-exponential decaying data, or in case of probability distributions need to be approximated, e.g. in case the data belong to Binomial, Exponential, Poisson, Hypergeometric or Gaussian distributions. As a convincing example the reader can see the results in [14, Figures 1 and 2] showing the exponential-reproduction capabilities of HP-splines. Particularly, [14, Figures 1] refers to data taken from the exponential function $e^{-\alpha x}$ while [14, Figures 2] to data from the function $xe^{-\alpha x}$. They are both examples of situation where HP-splines are more suitable than P-splines and give us an important information: in case we are dealing with data coming from specific exponential functions that are not corrupted by high noise, HP-splines are very good models. And this can also be the case of experimental data sets as Figure 8 shows. Nevertheless, even if the HP-spline derivation is not more complicated than the one of P-splines (see [11] and [14]), an additional and effective strategy to select the frequency parameter α, is required. Hence, the goal of this paper is to discuss a way to identify the HP-splines frequency parameter α from the data.

Our idea is to look at (1) with the penalty in (4), as a Tikhonov regularization problem in general form and use a result concerning the sensitivity of the model with respect to perturbation on the data. Obviously, the quantity expressing this sensitivity depends on both λ and α. Denoting this quantity with $\kappa_{\alpha,\lambda}$, our idea is to select the optimal frequency parameter α by minimizing $\kappa_{\alpha,\lambda}$. To this purpose, we define an explicit piecewise expression for the HB-basis functions in terms of α and then estimate the norms of the matrices involved in the determination of the minimum. This is particularly important in case the smoothing parameter λ is not set via a L-curve approach. Based on $\kappa_{\alpha,\lambda}$ or on its estimation $\tilde{\kappa}_{\alpha,\lambda}$, we provide an efficient *algorithm for the parameter selection* and show its effectiveness with several examples.

At this point it is important to mention that the analysis of our HP-spline model is not jet completed: the selection of the B-spline knots, the interrelation knots-data and the lack of symmetry of the proposed penalty are relevant and critical aspects worth to be considered.

The organization of the paper is as follows: in Section 2 we look at (1) with the penalty in (4) as a Tikhonov regularization problem in general form and recall a theorem investigating its sensitivity for the computation of the spline coefficients. In Section 3 we propose an estimate of the quantity that measures the sensitivity with respect to perturbation on the data. Then, in Section 4 we propose two possible algorithms for the frequency parameter selection. Numerical experiments are presented in Section 5 while Section 6 summarizes the proposed results. Concludes the paper an Appendix where the piecewise expression for the HB-splines in terms of α is provided.

2. HP-splines as a Tikhonov regularization problem

The hyperbolic-polynomial spline model we consider in this paper is made of segments in the four-dimensional space $\mathbb{E}_{4,\alpha}$ in (3). Given the data points (x_i, y_i), $i = 1, \ldots, m$, with $x_i \leq x_{i+1}$, and the uniform knot partition $\Xi := \{x_1 \equiv \xi_1 < \xi_2 \cdots < \xi_n \equiv x_m\}$ with knots distance h, we denote by $\{B_0^\alpha, \cdots, B_{n+1}^\alpha\}$ a HB-spline basis of the spline space that can be constructed as in [13] or as in [15] (for further details see Appendix). It consists of bell-shaped C^2-regular piecewise functions with segments in the space $\mathbb{E}_{4,\alpha}$, that have a compact support identified by 5 consecutive knots (see Fig. 1 left). Expressing the spline in terms of HB-splines, the HP-spline approximating the given data is obtained by solving the minimization problem

$$\arg \min_{\mathbf{a} \in \mathbb{R}^{n+2}} \sum_{i=1}^{m} w_i \left(y_i - \sum_{j=0}^{n+1} a_j B_j^\alpha(x_i) \right)^2 + \lambda^2 \sum_{j=2}^{n+1} \left((\Delta_2^{h,\alpha} \mathbf{a})_j \right)^2, \tag{5}$$

where the minimum is with respect to the HB-splines coefficients $\mathbf{a} = (a_j)_{j=0}^{n+1}$, $w_1, \ldots, w_m$, are non-zero weights, $\Delta_2^{h,\alpha}$ is the difference operator in (4). It is not difficult to see that the coefficient vector of the HP-spline

$$s_{\alpha,\lambda}(x) := \sum_{j=0}^{n+1} a_j B_j^\alpha(x),$$

approximating the data points (x_i, y_i), $i = 1, \ldots, m$, is the solution of the system of normal equations,

$$\left(\mathbf{B}_{h\alpha}^T \mathbf{W} \mathbf{B}_{h\alpha} + \lambda^2 (\mathbf{D}_{h\alpha})^T \mathbf{D}_{h\alpha} \right) \mathbf{a} = \mathbf{B}_{h\alpha}^T \mathbf{W} \mathbf{y}, \tag{6}$$

where $\mathbf{y} = (y_1, \ldots, y_m)^T \in \mathbb{R}^m$, $\mathbf{W} \in \mathbb{R}^{m \times m}$ is a diagonal matrix with diagonal entries $w_1, \ldots, w_m$, $\mathbf{D}_{h\alpha} \in \mathbb{R}^{n \times (n+2)}$, is the three-banded *difference* matrix

$$\mathbf{D}_{h\alpha} = \begin{bmatrix} 1 & -2e^{-\alpha h} & e^{-2\alpha h} & 0 & \cdots & 0 \\ 0 & 1 & -2e^{-\alpha h} & e^{-2\alpha h} & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \cdots & \vdots \\ \vdots & \vdots & \vdots & 1 & -2e^{-\alpha h} & e^{-2\alpha h} \end{bmatrix}, \tag{7}$$

and $\mathbf{B}_{h\alpha} \in \mathbb{R}^{m\times(n+2)}$, is the *collocation* matrix with elements

$$\mathbf{B}_{h\alpha} := \begin{bmatrix} B_0^\alpha(x_1) & B_1^\alpha(x_1) & \cdots & B_{n+1}^\alpha(x_1) \\ B_0^\alpha(x_2) & B_1^\alpha(x_2) & \cdots & B_{n+1}^\alpha(x_2) \\ \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \vdots \\ B_0^\alpha(x_{m-1}) & B_1^\alpha(x_{m-1}) & \cdots & B_{n+1}^\alpha(x_{m-1}) \\ B_0^\alpha(x_m) & B_1^\alpha(x_m) & \cdots & B_{n+1}^\alpha(x_m) \end{bmatrix}. \tag{8}$$

The matrix $\mathbf{B}_{h\alpha}$ is a banded matrix whose bandwidth is inherited by the HB-spline locality and depends on the relation among HB-spline knots and data abscissae. In spite of the bandwidth of $\mathbf{B}_{h\alpha}$, the symmetric matrix $(\mathbf{B}_{h\alpha})^T\mathbf{W}\mathbf{B}_{h\alpha} \in \mathbb{R}^{(n+2)\times(n+2)}$ is with band-width at most 7 as in case of cubic polynomial B-splines. To see it, we recall that the support of any B_k^α, $k = 0, \dots n+1$ is identified by 5 consecutive knots, say $\xi_{k-2},\ \xi_{k-1},\ \xi_k,\ \xi_{k+1},\ \xi_{k+2}$. Since

$$\left((\mathbf{B}_{h\alpha})^T\mathbf{W}\mathbf{B}_{h\alpha}\right)_{\ell,j} = \sum_{i=1}^{m} B_\ell^\alpha(x_i) w_i B_j^\alpha(x_i), \quad \ell, j = 0, \dots n+1,$$

it follows that $\left((\mathbf{B}_{h\alpha})^T\mathbf{W}\mathbf{B}_{h\alpha}\right)_{\ell,j} \neq 0$ for ℓ, j such that $\mathrm{supp}(B_\ell^\alpha) \cap \mathrm{supp}(B_j^\alpha) \neq \emptyset$ which means for at most the 7 consecutive indices $\ell \in \{j-3, j-2, \dots, j+2, j+3\}$. For simplicity and without loss of generality, we

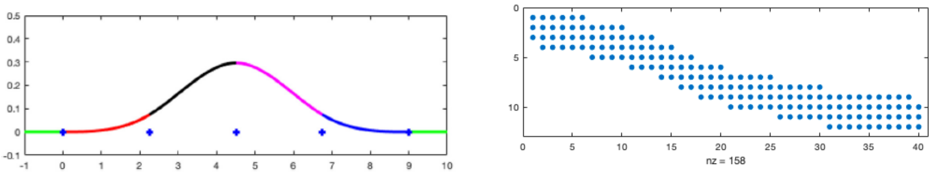

Figure 1: HB spline (left) and the $\mathbf{B}_{h\alpha}^T$ structure (right).

assume that the matrix $\mathbf{W}$ is the identity matrix.
Looking at (6) as a Tikhonov regularization problem in general form,

$$\min_{\mathbf{a}\in\mathbb{R}^{n+2}} \|\mathbf{B}_{h\alpha}\mathbf{a} - \mathbf{y}\|_2^2 + \lambda^2\|\mathbf{D}_{h\alpha}\mathbf{a}\|_2^2 \tag{9}$$

we can use the argument in [24, page 16] and in [6, Appendix B] to conclude that the solution exists and it is unique and it is given by:

$$\mathbf{a}_{\alpha,\lambda} = \mathbf{B}_{\alpha,\lambda}^\sharp \mathbf{y}, \tag{10}$$

where

$$\mathbf{B}_{\alpha,\lambda}^\sharp = \left(\mathbf{B}_{h\alpha}^T\mathbf{B}_{h\alpha} + \lambda^2(\mathbf{D}_{h\alpha})^T\mathbf{D}_{h\alpha}\right)^{-1}\mathbf{B}_{h\alpha}^T, \tag{11}$$

is the *regularized inverse matrix*.

Remark 2.1. It is worth noting that, unless the smoothing parameter λ is a priori fixed, in spite of the specific method of selection, it always strongly depends on the data and on the spline space frequency α. Therefore, it should be denoted as $\lambda(\alpha, \mathbf{x}, \mathbf{y})$. But, for shortness, we will refer to it just as λ.
As for the model definition when α approaches to extreme values, our algorithm does not allow the search of a very large α but presents an issue when $\alpha \to 0$. In the latter case, the use of a P-spline instead of an HP-spline would be the simple recommendation. However, in Section 5 we propose to use a threshold acting as a lower bound for $|\alpha|$ around 0. For interested readers, we mention that to deal with $\alpha \to 0$ other stable techniques can be found in the recent works [16, 17] and references therein.

2.1. Sensitivity with respect to data perturbation

It is well known (for details see [18]) that the numerical solution of the Tikhonov regularization problem in (6) with $\mathbf{W} = \mathbf{I}$, can be expressed in terms of the GSVD of the two matrices $(\mathbf{B}_{h\alpha}, \mathbf{D}_{h\alpha})$. The GSVD of a couple of matrices is a generalization of the SVD consisting is the simultaneous decomposition of both matrices in orthonormal and diagonal factors as

$$\mathbf{B}_{h\alpha} = \mathbf{U}_{h\alpha} \begin{pmatrix} \mathbf{\Sigma}_{h\alpha} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{h\alpha} \end{pmatrix} \mathbf{X}_{h\alpha}^{-1}, \qquad \mathbf{D}_{h\alpha} = \mathbf{V}_{h\alpha} \begin{pmatrix} \mathbf{N}_{h\alpha} & \mathbf{0} \end{pmatrix} \mathbf{X}_{h\alpha}^{-1}, \tag{12}$$

where $\mathbf{U}_{h\alpha} \in \mathbb{R}^{m\times(n+2)}$, $\mathbf{I}_{h\alpha} \in \mathbb{R}^{2\times 2}$ and $\mathbf{V}_{h\alpha} \in \mathbb{R}^{n\times n}$ are orthonormal, $\mathbf{X}_{h\alpha} \in \mathbb{R}^{(n+2)\times(n+2)}$ is nonsingular, and $\mathbf{\Sigma}_{h\alpha}$ and $\mathbf{N}_{h\alpha}$ are $n \times n$ diagonal matrices $\mathbf{\Sigma}_{h\alpha} = diag(\sigma_1, \ldots, \sigma_n)$, $\mathbf{N}_{h\alpha} = diag(\nu_1, \ldots, \nu_n)$, with diagonal elements non-negative and ordered

$$0 \leq \sigma_1 \leq \ldots \leq \sigma_n \leq 1, \qquad 0 < \nu_n \leq \ldots \leq \nu_1 \leq 1. \tag{13}$$

Based on a classical perturbation bound for Tikhonov regularization (see [18, Theorem 5.1.1]) the condition number of the least square problem (9) can be expressed as a function of both the smoothing and the frequency parameters λ and α, according to the following result, whose proof follows directly from [18, Theorem 5.1.1].

Theorem 2.1. Let (9) be a Tikhonov problem in general form. Let $\mathbf{X}_{h\alpha}$ be the factor of the GSVD of $(\mathbf{B}_{h\alpha}, \mathbf{D}_{h\alpha})$ as in (12) and $cond(\mathbf{X}_{h\alpha})$ its 2-norm condition number. Let $\mathbf{a}_{\alpha,\lambda}$ and $\tilde{\mathbf{a}}_{\alpha,\lambda}$ be the solutions of the Tikhonov problem in general form, and of its perturbed version, respectively given by

$$\min_{\mathbf{a}\in\mathbb{R}^{n+2}} \|\mathbf{B}_{h\alpha}\mathbf{a} - \mathbf{y}\|_2^2 + \lambda^2\|\mathbf{D}_{h\alpha}\mathbf{a}\|_2^2 \quad \text{and} \quad \min_{\mathbf{a}\in\mathbb{R}^{n+2}} \|\tilde{\mathbf{B}}_{h\alpha}\mathbf{a} - \tilde{\mathbf{y}}\|_2^2 + \lambda^2\|\mathbf{D}_{h\alpha}\mathbf{a}\|_2^2. \tag{14}$$

Defining $\mathbf{e} = \mathbf{y} - \tilde{\mathbf{y}}$, $\epsilon = \|\mathbf{B}_{h\alpha} - \tilde{\mathbf{B}}_{h\alpha}\|_2/\|\mathbf{B}_{h\alpha}\|_2$, $\mathbf{y}_{\alpha,\lambda} = \mathbf{B}_{h\alpha}\mathbf{a}_{\alpha,\lambda}$, $\mathbf{r}_{\alpha,\lambda} = \mathbf{y} - \mathbf{y}_{\alpha,\lambda}$, and

$$\kappa_{\alpha,\lambda} = \|\mathbf{B}_{h\alpha}\|_2\|\mathbf{X}_{h\alpha}\|_2/\lambda, \tag{15}$$

under the assumption $\epsilon\kappa_{\alpha,\lambda} < 1$ it results that

$$\frac{\|\mathbf{a}_{\alpha,\lambda} - \tilde{\mathbf{a}}_{\alpha,\lambda}\|_2}{\|\mathbf{a}_{\alpha,\lambda}\|_2} \leq \frac{\kappa_{\alpha,\lambda}}{1 - \epsilon\kappa_{\alpha,\lambda}} \left((1 + cond(\mathbf{X}_{h\alpha}))\epsilon + \frac{\|\mathbf{e}\|_2}{\|\mathbf{y}_{\alpha,\lambda}\|_2} + \epsilon\kappa_{\alpha,\lambda}\frac{\|\mathbf{r}_{\alpha,\lambda}\|_2}{\|\mathbf{y}_{\alpha,\lambda}\|_2} \right), \quad 0 < \lambda \leq 1 \tag{16}$$

Remark 2.2. We remark that (16) is a general error bound on $\mathbf{a}_{\alpha,\lambda}$. In this paper we assume $\epsilon = 0$, i.e. that the perturbation on $\mathbf{B}_{h\alpha}$ is negligible, and therefore (16) becomes the tighter bound:

$$\frac{\|\mathbf{a}_{\alpha,\lambda} - \tilde{\mathbf{a}}_{\alpha,\lambda}\|_2}{\|\mathbf{a}_{\alpha,\lambda}\|_2} \leq \kappa_{\alpha,\lambda}\frac{\|\mathbf{e}\|_2}{\|\mathbf{y}_{\alpha,\lambda}\|_2}. \tag{17}$$

3. Estimate of $\kappa_{\alpha,\lambda}$

This section is to discuss an estimate of $\kappa_{\alpha,\lambda} = \|\mathbf{B}_{h\alpha}\|_2\|\mathbf{X}_{h\alpha}\|_2/\lambda$, the quantity expressing the sensitivity of the solution of the Tikhonov regularization problem in general form depending on both λ and α. While, in general, a correct HP-spline identification requires the reciprocal updating of α and λ, our idea is to first identify α and then λ by the help of some criteria for setting the smoothing parameter. Unless the smoothing parameter is set via a L-curve approach (see [7] for a complete discussion about the L-curve method), to reduce the computational cost associated with $\kappa_{\alpha,\lambda}$ we propose a way to estimate $\kappa_{\alpha,\lambda}$, say $\tilde{\kappa}_{\alpha,\lambda}$, based on an approximation of $\|\mathbf{B}_{h\alpha}\|_2$ and $\|\mathbf{X}_{h\alpha}\|_2$.

The following Lemma gives a bound for the 2-norm of $\mathbf{B}_{h\alpha}$, depending on both α and h.

Lemma 3.1. The 2-norm of the collocation matrix $\mathbf{B}_{h\alpha}$ in (8), is bounded by:

$$\|\mathbf{B}_{h\alpha}\|_2 \leq \sqrt{m}\|\mathbf{B}_{h\alpha}\|_\infty \leq 4\sqrt{m}\,\frac{\left((e^{\alpha\, 2h} - e^{-\alpha\, 2h}) - 4\alpha\, h\right)}{4(\alpha\, h)^3}.$$

Proof. Using Proposition Appendix A.3, we easily see that the rows of the matrix $\mathbf{B}_{h\alpha}$, depend on the HB-splines values at data points. Now, since each HB-spline $B_j^\alpha = B_0^\alpha(\cdot - jh)$ is supported in the interval $[\xi_{j-2},\ \xi_{j+2}]$, at most 4 HB-splines are non zero in a data point. In consideration that all B_j^α are shifted version of the same bell-shaped function whose maximum value $M_{h\alpha}$ is reached at the central knot, from (A.5) we easily deduce that

$$\begin{aligned} M_{h\alpha} &= B_{h\alpha}^h(2h) \\ &= \left(-4\cosh(0) + \frac{4\sinh(0)}{h\alpha} + \frac{1}{h\alpha} 2\sinh(\alpha 2h)\right)/4(\alpha\, h)^2 \\ &= \left(-4 + \frac{1}{h\alpha}(e^{\alpha\, 2h} - e^{-\alpha\, 2h})\right)/4(\alpha\, h)^2. \end{aligned} \tag{18}$$

Hence, taking into account that $\|\mathbf{B}_{h\alpha}\|_\infty = \max_{1\le i\le m} \sum_{j=1}^{n+2} |b_{ij}|$, with

$$b_{ij} = B_j^\alpha(x_i) = B_0^\alpha(x_i - jh),\ i = 1, \dots, m,\ j = 1, \cdots, n+2.$$

we easily conclude that

$$\|\mathbf{B}_{h\alpha}\|_\infty \le 4\, M_{h\alpha}.$$

By the equivalence of the matrix norms (see [19, eq. (2.3.12)], for example) the claim follows. $\square$

Now we search for an estimate for $\|\mathbf{X}_{h\alpha}\|_2$, taking into account that it is

$$\|\mathbf{D}_{h\alpha}^\dagger\|_2 = \|\mathbf{D}_{h\alpha}^T \left(\mathbf{D}_{h\alpha}\mathbf{D}_{h\alpha}^T\right)^{-1}\|_2 \le \|\mathbf{D}_{h\alpha}^T\|_2 \, \| \left(\mathbf{D}_{h\alpha}\mathbf{D}_{h\alpha}^T\right)^{-1}\|_2.$$

Following [18], we assume:

$$\|\mathbf{X}_{h\alpha}\|_2 \le \|\mathbf{D}_{h\alpha}^\dagger\|_2 \tag{19}$$

so we can conclude that

$$\|\mathbf{X}_{h\alpha}\|_2 \le \|\mathbf{D}_{h\alpha}^T\|_2 \, \| \left(\mathbf{D}_{h\alpha}\mathbf{D}_{h\alpha}^T\right)^{-1}\|_2.$$

Setting $a := e^{-\alpha\, h} > 0$ we have that

$$\mathbf{D}_{h\alpha}(\mathbf{D}_{h\alpha})^T = \begin{bmatrix} 1+4a^2+a^4 & -2a-2a^3 & a^2 & 0 & \cdots & 0 \\ -2a-2a^3 & 1+4a^2+a^4 & -2a-2a^3 & a^2 & \cdots & 0 \\ a^2 & -2a-2a^3 & 1+4a^2+a^4 & -2a-2a^3 & a^2 & 0 \\ 0 & a^2 & -2a-2a^3 & 1+4a^2+a^4 & -2a-2a^3 & a^2 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & a^2 & -2a-2a^3 & 1+4a^2+a^4 & -2a-2a^3 \\ 0 & 0 & 0 & a^2 & -2a-2a^3 & 1+4a^2+a^4 \end{bmatrix}, \tag{20}$$

is a Toeplitz, symmetric, pentadiagonal matrix such that $\| \left(\mathbf{D}_{h\alpha}(\mathbf{D}_{h\alpha})^T\right)^{-1}\|_2 = \frac{1}{\lambda_{min}}$ with λ_{min} the minimal eigenvalue of $\mathbf{D}_{h\alpha}(\mathbf{D}_{h\alpha})^T$. If we associate to $\mathbf{D}_{h\alpha}(\mathbf{D}_{h\alpha})^T$ its trigonometric *symbol*

$$g(\theta) = (1+4a^2+a^4) - 4(a+a^3)\cos(\theta) + 2a^2\cos(2\theta) = 4a^2\cos^2(\theta) - 4a(1+a^2)\cos(\theta) + (1+2a^2)^2,$$

we see that

$$g(\theta) \ge 0 \quad \text{and} \quad g(\theta) = 0 \quad \Leftrightarrow \quad \cos(\theta) = \frac{1+a^2}{2a}.$$

Next, we use the 'interlacing' result in [20, Section 4], to deduce that λ_{min} is bounded from below by

$$q(a) = \min\left\{ g\left(\frac{2\pi}{n+3}\right),\ g\left(\frac{\pi}{n+3}\right)\right\}.$$

It is easy to see that $g(a) \neq 0$: Indeed for $a \neq 1$

$$g\left(\frac{2\pi}{n+3}\right) \neq 0 \quad \Leftrightarrow \quad \cos\left(\frac{2\pi}{n+3}\right) \neq \frac{1+a^2}{2a} = 1 + \frac{(1-a)^2}{2a} > 1,$$

as well as

$$g\left(\frac{\pi}{n+3}\right) \neq 0 \quad \Leftrightarrow \quad \cos\left(\frac{\pi}{n+3}\right) \neq \frac{1+a^2}{2a} = 1 + \frac{(1-a)^2}{2a} > 1.$$

For $a = 1$, since $\frac{2\pi}{n+3}$ and $\frac{\pi}{n+3}$ are not multiple of $\frac{\pi}{2}$, it easily follows that both $\cos(\frac{2\pi}{n+3}) \neq 1$ and $\cos(\frac{\pi}{n+3}) \neq 1$ implying $g(\frac{2\pi}{n+3}) \neq 0$ and $g(\frac{\pi}{n+3}) \neq 0$. In conclusion, we have that

$$\frac{1}{\lambda_{min}} \leq \frac{1}{q(a)}.$$

Now, taking into consideration that

$$\|\mathbf{D}_{h\alpha}\|_2 \leq \sqrt{\|\mathbf{D}_{h\alpha}\|_1 \, \|\mathbf{D}_{h\alpha}\|_\infty} = (a+1)^2,$$

from (19), we arrive at

$$\|\mathbf{D}_{h\alpha}^{\dagger}\|_2 \leq \|\mathbf{D}_{h\alpha}^T\|_2 \, \| \left(\mathbf{D}_{h\alpha}\mathbf{D}_{h\alpha}^T\right)^{-1} \|_2 \leq \frac{(a+1)^2}{q(a)}.$$

All considered, our estimate for $\tilde{\kappa}_{\alpha,\lambda}$ is given by

$$\tilde{\kappa}_{\alpha,\lambda} = \frac{1}{\lambda}\left(\sqrt{m}\frac{((e^{2\alpha\, h} - e^{-2\alpha\, h}) - 4\alpha\, h)}{(\alpha\, h)^3}\right) \cdot \frac{(e^{-\alpha\, h}+1)^2}{q(e^{-\alpha\, h})}, \tag{21}$$

which is numerically proven to be a very good estimate (see the next Section).

4. Two algorithms for the selection of the frequency α of HP-splines

This section is to discuss two algorithms for the frequency parameter selection derived by minimizing $\kappa_{\alpha,\lambda}$ and $\tilde{\kappa}_{\alpha,\lambda}$ respectively. Referring to the first algorithm, given a data set and a suitable frequency interval, say $[\alpha_{min}, \alpha_{max}]$, for $\alpha \in [\alpha_{min}, \alpha_{max}]$, we first, compute the matrices $\mathbf{B}_{h\alpha}$ and $\mathbf{D}_{h\alpha}$, compute $\mathbf{X}_{h\alpha}$ via their GSVD, and then the regularization parameter λ (depending on α) by the L-curve method. With the couple (α, λ) we compute $\kappa_{\alpha,\lambda}$ as in (15). The value $\arg\min_\alpha \kappa_{\alpha,\lambda}$ is the *optimal* frequency parameter.

The simplest possible procedure for minimizing $\kappa_{\alpha,\lambda}$, consists in the construction of a look-up table based on a possible set of (α, λ)-values, and then searching for the minimum in that table. This naive approach requires the choice of the α searching interval and of its *discretization step*. Since we have verified that the searching interval for α affects the result more than the *step*, given a data set $(x_i, y_i)_{i=1}^m$ we propose to consider searching intervals depending on the data behaviour as follows:

$$[\alpha_{min}, \alpha_{max}] = \begin{cases} [\alpha_{min}, -\tau) & \text{if } y_m < y_1 \\ (\tau, \alpha_{max}] & \text{if } y_m > y_1, \end{cases} \tag{22}$$

where α_{min} and α_{max} are such that $\alpha_{fit} \in (\alpha_{min}, \alpha_{max})$, with α_{fit} resulting from nonlinear least-squares regression of the data in the space $\mathbb{E}_{4,\alpha}$ and τ is a suitable threshold for an admissible α. To be more precise, the parameter α_{fit} is set as $\alpha_{fit} = |c_3| sign(y_m - y_1)$ with c_3 obtained via nonlinear least-squares approximation of the data by the 5-parameters function $g(\mathbf{c}, x) = c_1 \cdot x^{c_4} \cdot e^{c_3 x} + c_2 \cdot x^{c_5} \cdot e^{-c_3 x}$. The mentioned α_{fit} can be computed by the MATLAB function `lsqnonneg`. As for the threshold τ, our proposal is to set it as $\tau = 1.0e-5$ in consideration of the several numerical tests we have conducted. A simple test is also reported in Subsection 5.4 showing that only for $|\alpha| > \tau = 1.0e-5$ a reliable approximation is granted.

This idea is summarized in the following algorithm.

Algorithm 1 Algorithm for data driven selection of α by $\kappa_{\alpha,\lambda}$

1: set $\alpha_{fit} \leftarrow$ Fixed initial guess
2: set $J = [\alpha_{min} : step : \alpha_{max}]$ by (22) $\leftarrow$ Search interval with step-size *step*
3: **for** $i = 1$ to length(J) **do**
4: $\quad\alpha = J(i)$
5: $\quad$compute $\mathbf{B}_{h\alpha}$ and $\mathbf{D}_{h\alpha}$
6: $\quad$compute $\mathbf{X}_{h\alpha}$ by GSVD of $(\mathbf{B}_{h\alpha}, \mathbf{D}_{h\alpha})$
7: $\quad$compute λ by L-curve
8: $\quad$compute the entry $\kappa_{\alpha,\lambda}$
9: $\quad$set $T(i) = \kappa_{\alpha,\lambda}$
10: **end for**
11: find $\alpha = \arg\min\{T\}$

Algorithm 2 Algorithm for data driven selection of α by $\tilde{\kappa}_{\alpha,\lambda}$

1: set $\alpha_{fit} \leftarrow$ Fixed initial guess
2: set $J = [\alpha_{min} : step : \alpha_{max}]$ by (22) $\leftarrow$ Search interval with step-size *step*
3: **for** $i = 1$ to length(J) **do**
4: $\quad\alpha = J(i)$
5: $\quad$compute λ
6: $\quad$compute the entry $\tilde{\kappa}_{\alpha,\lambda}$
7: $\quad$set $T(i) = \tilde{\kappa}_{\alpha,\lambda}$
8: **end for**
9: find $\alpha = \arg\min\{T\}$

As an alternative, in the step 8 of Algorithm 1, we propose the computation of $\tilde{\kappa}_{\alpha,\lambda}$ as in (21) instead of $\kappa_{\alpha,\lambda}$. From the discussion in the previous Section, we know that $\tilde{\kappa}_{\alpha,\lambda}$ is a very reasonable estimate for the sensitivity factor of the model with respect to perturbation on the data and, more importantly, its computation doesn't require $\mathbf{B}_{h\alpha}, \mathbf{D}_{h\alpha}$ and their GSVD. This is particularly important in case the regularization parameter is computed via different criteria than the L-curve like GCV, for example. A possible algorithm for selecting the α minimizing $\tilde{\kappa}_{\alpha,\lambda}$ follows. We continue this section by presenting a motivating example, where $\tilde{\kappa}_{\alpha,\lambda}$ behaves *just* like an upper bound for $\kappa_{\alpha,\lambda}$ and where the minimum of both $\kappa_{\alpha,\lambda}$ and $\tilde{\kappa}_{\alpha,\lambda}$, is reached at quite the same $\alpha-$value. Even if this behaviour is experimentally verified mostly for data with an exponential trend, the next section shows that the minimization of $\tilde{\kappa}_{\alpha,\lambda}$ can be effective also for data that belong to functions with a different trend. The example consider the approximation of a data set extracted from a pure exponential function. Obviously, for this type of data, the best possible frequency parameter of the spline space α, is *just* the frequency parameter of the generating function. To recover it, we first set the optimal frequency parameter by minimizing $\kappa_{\alpha,\lambda}$, then, we set α by minimizing $\tilde{\kappa}_{\alpha,\lambda}$. As evident in Figure 2, minimization of both $\kappa_{\alpha,\lambda}$ and of $\tilde{\kappa}_{\alpha,\lambda}$ results in a good strategy to identify the frequency parameter α. Since the approach based on the minimization of $\tilde{\kappa}_{\alpha,\lambda}$ is certainly cheaper, Algorithm 2 is the one to be preferred.

A motivating example 4.1. Let $(x_i, y_i)_{i=1}^{m=40}$, be a data set with x_i randomly distributed abscissae in $[0, 5]$, $y_i = f(x_i)$, $f(x) = e^{-x}$. The spline space we use is based on $n = 11$ knots uniformly distributed in $[0, 5]$ (that is $h = 0.5$). To select α we let it vary in the interval $(-1.5, -0.1)$ and compute both $\kappa_{\alpha,\lambda}$ and $\tilde{\kappa}_{\alpha,\lambda}$. Figure 2 displays their values and shows that the minimum of both $\kappa_{\alpha,\lambda}$ and $\tilde{\kappa}_{\alpha,\lambda}$ is reached exactly at $\alpha = -1$ which is, indeed, *the best* possibile value of α describing the exponential data trend. For this data set we also present a table showing, for different values of α, the relative errors of the spline $s_{\alpha,\lambda}$ both with respect to the data and the original function. In the first case, for $\mathbf{x} = (x_i)_{i=1}^{40}$ and $\mathbf{y} = (y_i)_{i=1}^{40}$ we compute

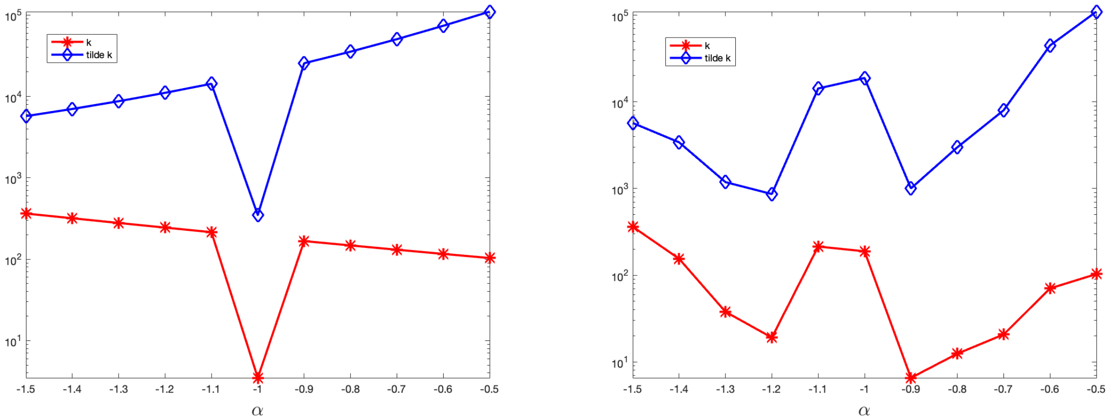

Figure 2: The estimate $\tilde{\kappa}_{\alpha,\lambda}$ (blue '$\diamond$') and $\kappa_{\alpha,\lambda}$ (red '*') for different α values; $\sigma = 0$ (left), and $\sigma = 1.0e - 2$ (right).

the quantity

$$\delta_{\alpha,\lambda} = \frac{\|s_{\alpha,\lambda}(\mathbf{x}) - \mathbf{y}\|_2}{\|\mathbf{y}\|_2}, \tag{23}$$

while in the second one we compute the quantity

$$\varepsilon_{\alpha,\lambda} = \frac{\|s_{\alpha,\lambda}(\mathbf{v}) - f(\mathbf{v})\|_2}{\|f(\mathbf{v})\|_2}, \tag{24}$$

for uniformly distributed points $\mathbf{v} = (v_i)_{i=1}^{100}$ with $v_1 = x_1$, $v_{100} = x_{40}$. We initially consider exact data and report the results in Table 1 (top), then we repeat the experiment assuming the data are affected by Gaussian noise with standard deviation equal to $\sigma = 1.0e - 2$; the results in Table 1 (bottom) show that the criteria to select the frequency parameter work; in fact, the quite similar frequency value, $\alpha = -0.9$ and $\alpha = -1.2$ for which $\kappa_{\alpha,\lambda}$ and $\tilde{\kappa}_{\alpha,\lambda}$ are respectively the smallest, define a HP-spline that furnishes a good accuracy in the approximation of f.

Before we conclude this section some numerical remarks, synthesis of the many conducted experiments, are worthwhile to be made.

Remark 4.1.

i) From Theorem 2.1 we know that the quantity $\kappa_{\alpha,\lambda}$ plays the role of a condition number for the Tikhonov regularized solution and its smallest value is reached by the biggest λ. This could suggest that minimizing with respect to both α and λ may improve the accuracy on the solution. But, increasing λ also increases the regularization error (as mentioned already in [18]). This is why a double tabulation with respect both α and λ is not recommended, providing a too small (and not best) choice for $\kappa_{\alpha,\lambda}$ (and $\tilde{\kappa}_{\alpha,\lambda}$).

ii) Another remark concerns the computed λ-values. It's worth noting that, in all the tests, the algorithm works well also when λ become greater than one and therefore even in case the assumptions of Theorem 2.1 are not satisfied.

iii) As a possible searching criterion for α, capable of capturing the trend of assigned *noisy* data, one could consider the minimization of the *computational error estimate*: $\Gamma_{\alpha,\lambda} = \tilde{\kappa}_{\alpha,\lambda} \cdot \frac{\|\mathbf{e}\|_2}{\|\mathbf{y}_{\alpha,\lambda}\|_2}$.

5. Numerical results

This section presents some of the many numerical experiments we have conducted to test our frequency parameter selection strategies. All experiments were carried out on a Intel(R) Core(TM) i5, 1.8 GHz

$\sigma = 0$					
α	λ	$\kappa_{\alpha,\lambda}$	$\tilde{\kappa}_{\alpha,\lambda}$	$\delta_{\alpha,\lambda}$	$\varepsilon_{\alpha,\lambda}$
-1.5000e+00	1.7470e-02	3.6377e+02	5.7250e+03	2.5433e-04	3.1873e-04
-1.4000e+00	1.8912e-02	3.1826e+02	7.0113e+03	1.7647e-04	2.1320e-04
-1.3000e+00	2.0473e-02	2.7876e+02	8.7285e+03	1.0746e-04	1.2564e-04
-1.2000e+00	2.2161e-02	2.4453e+02	1.1064e+04	5.1607e-05	5.8603e-05
-1.1000e+00	2.3988e-02	2.1487e+02	1.4303e+04	1.3910e-05	1.5389e-05
$\boxed{\textbf{-1.0000e+00}}$	2.1574e+00	$\boxed{\textbf{2.2767e+00}}$	$\boxed{\textbf{2.2741e+02}}$	2.6100e-15	2.9078e-15
-9.0000e-01	2.8098e-02	1.6690e+02	2.5560e+04	1.6047e-05	1.6979e-05
-8.0000e-01	3.0406e-02	1.4757e+02	3.5455e+04	6.8651e-05	7.1253e-05
-7.0000e-01	3.2899e-02	1.3076e+02	5.0482e+04	1.6469e-04	1.6794e-04
-6.0000e-01	3.5592e-02	1.1612e+02	7.3727e+04	3.1116e-04	3.1216e-04
-5.0000e-01	3.8500e-02	1.0335e+02	1.0998e+05	5.1495e-04	5.0880e-04

$\sigma = 10^{-2}$					
α	λ	$\kappa_{\alpha,\lambda}$	$\tilde{\kappa}_{\alpha,\lambda}$	$\delta_{\alpha,\lambda}$	$\varepsilon_{\alpha,\lambda}$
-1.5000e+00	1.7528e-02	3.6256e+02	5.7060e+03	1.9976e-03	6.7091e-03
-1.4000e+00	3.8837e-02	1.5498e+02	3.4142e+03	2.0731e-03	6.4206e-03
-1.3000e+00	1.5067e-01	3.7878e+01	1.1860e+03	2.5072e-03	6.0807e-03
$\boxed{\textbf{-1.2000e+00}}$	2.8362e-01	1.9107e+01	$\boxed{\textbf{8.6448e+02}}$	2.5243e-03	6.0240e-03
-1.1000e+00	2.4040e-02	2.1440e+02	1.4272e+04	2.0407e-03	6.5207e-03
-1.0000e+00	2.6021e-02	1.8876e+02	1.8855e+04	2.0497e-03	6.5001e-03
$\boxed{\textbf{-9.0000e-01}}$	7.1554e-01	$\boxed{\textbf{6.5541e+00}}$	1.0037e+03	2.4924e-03	6.0353e-03
-8.0000e-01	3.6074e-01	1.2438e+01	2.9884e+03	2.5376e-03	6.0538e-03
-7.0000e-01	2.0757e-01	2.0726e+01	8.0013e+03	2.5226e-03	6.1063e-03
-6.0000e-01	5.8644e-02	7.0478e+01	4.4746e+04	2.0933e-03	6.3905e-03
-5.0000e-01	3.8555e-02	1.0320e+02	1.0982e+05	2.0235e-03	6.6100e-03

Table 1: Test function $f(x) = e^{-x}$: numerical results for different α values; from top to bottom we set $\sigma = 0$ and $\sigma = 1.0e-2$.

processor, with a MATLAB® R2022b code available from the authors. The Tikhonov solution has been computed by means of the GSVD factorization which is also used to compute the smoothing parameter λ by L-curve, via Hansen package `Regularization Tools` [21] available at MATLAB Central File Exchange[1]. The use of GCV to compute the regularization parameter is also possible using the same toolbox.

Tests 1-5 consider a synthetic data set of type

$$(x_i, \tilde{y}_i)_{i=1,\dots,m}, \quad x_i \in [a, b] \quad \tilde{y}_i = f(x_i) + \sigma_i, \quad i = 1, \dots, m,$$

with x_i randomly distributed abscissae, f chosen from a database of functions, and ordinates $f(x_i)$ affected by Gaussian noise distributed with zero mean and standard deviation σ. The reliability of the described procedure is confirmed by the computation of the relative error on the solution as in (23) and in (24), at uniformly distributed points.

The function database we consider consists of a multi-exponential function f_1 (for which we expect the HP-spline to perform at the best) and of the non-exponential functions f_2, f_3, f_4 to prove the efficacy of the selection rule for the parameter α also when the data follow non-exponential trend and f_5 is to discuss about the approximation when $\alpha \to 0$:

1. $f_1(x) = e^{\frac{x}{2}} + \frac{x}{2}e^{-2x}$ in $[0, 5]$;
2. $f_2(x) = 1/\sqrt{1 + x^2}$ in $[0, 5]$;
3. $f_3(x) = log(x^2) + x^3 e^x$ in $[3, 7]$;
4. $f_4(x) = sin(x)cos(2x)$ in $[-3, 3]$;
5. $f_5(x) = 1/(x - 11)$ in $[0, 10]$.

The numerical results are reported in the Tables 2, 3, 4, 5. Every table displays the computed values of $\alpha, \lambda, \kappa_{\alpha,\lambda}$, and $\tilde{\kappa}_{\alpha,\lambda}$. The relative errors on the solution $\delta_{\alpha,\lambda}$ and $\varepsilon_{\alpha,\lambda}$ are computed as in (23) and (24) and reported in the rightmost columns. From the boldface value in every table, we see that the accuracy of the solution obtained by the corresponding HP-splines, in both cases, is comparable and satisfactory, as the relative errors in the last column confirm.
The last Test 6 is to compare the performances of HP-spline with respect to P-spline, on a real dataset proposed in [23].
For all tests, from 1 to 6, we use Algorithm 1 to select the frequency value α corresponding to the minimum value for $\kappa_{\alpha,\lambda}$, and Algorithm 2 to select the α corresponding to the minimum value for $\tilde{\kappa}_{\alpha,\lambda}$. We observe that, in all tests, the algorithm works well even in case $\lambda > 1$, that is when the hypothesis of Theorem 2.1 is violated

5.1. Test f_1

First we consider f_1 and the following problem setting: $n = 11$ splines knots uniformly distributed in $[0, 5]$, spacing $h = 0.5$ and $m = 40$ data points.The numerical results are reported in Table 2 for different values of σ. Fig. 3 compares $\kappa_{\alpha,\lambda}$ and $\tilde{\kappa}_{\alpha,\lambda}$ for different values of σ and shows that the minimum value is reached for the same α, both in case of $\sigma = 0$ and $\sigma \neq 0$.

5.2. Test f_2 and f_3

These two tests are to prove the reliability of the α-selection strategy in case of *non exponential* data. First, we consider f_2, $n = 11$ knots uniformly distributed in $[a, b] = [0, 5]$ with spacing $h = 0.5$, $m = 40$ data points and $\sigma = 1.0e-2$. Fig. 4 shows $\tilde{\kappa}_{\alpha,\lambda}$ and $\kappa_{\alpha,\lambda}$ for different values of $\alpha \in [-0.9, 0.9]$ (top). In the same figure, we report the HP-spline fitting $(x_i, \tilde{y}_i)_{i=1,\dots,m}, \tilde{y}_i = f_2(x_i) + \sigma_i$, $m = 40$, with α minimizing $\kappa_{\alpha,\lambda}$ (bottom,left) and $\tilde{\kappa}_{\alpha,\lambda}$ (bottom,right).

Then, we consider f_3, set $n = 9$ knots uniformly distributed in $[a, b] = [3, 7]$ with spacing $h = 0.5$, $m = 33$ data points and $\sigma = 1.0e-2$. Fig. 5 shows $\tilde{\kappa}_{\alpha,\lambda}$ and $\kappa_{\alpha,\lambda}$ for different values of $\alpha \in [0.1, 1.5]$ (top). In the same figure, we report the HP-spline fitting $(x_i, \tilde{y}_i)_{i=1,\dots,m}, \tilde{y}_i = f_3(x_i) + \sigma_i$, $m = 33$, with α minimizing $\kappa_{\alpha,\lambda}$ (bottom,left) and $\tilde{\kappa}_{\alpha,\lambda}$ (bottom,right).

[1] `https://www.mathworks.com/matlabcentral/fileexchange/52-regtools`

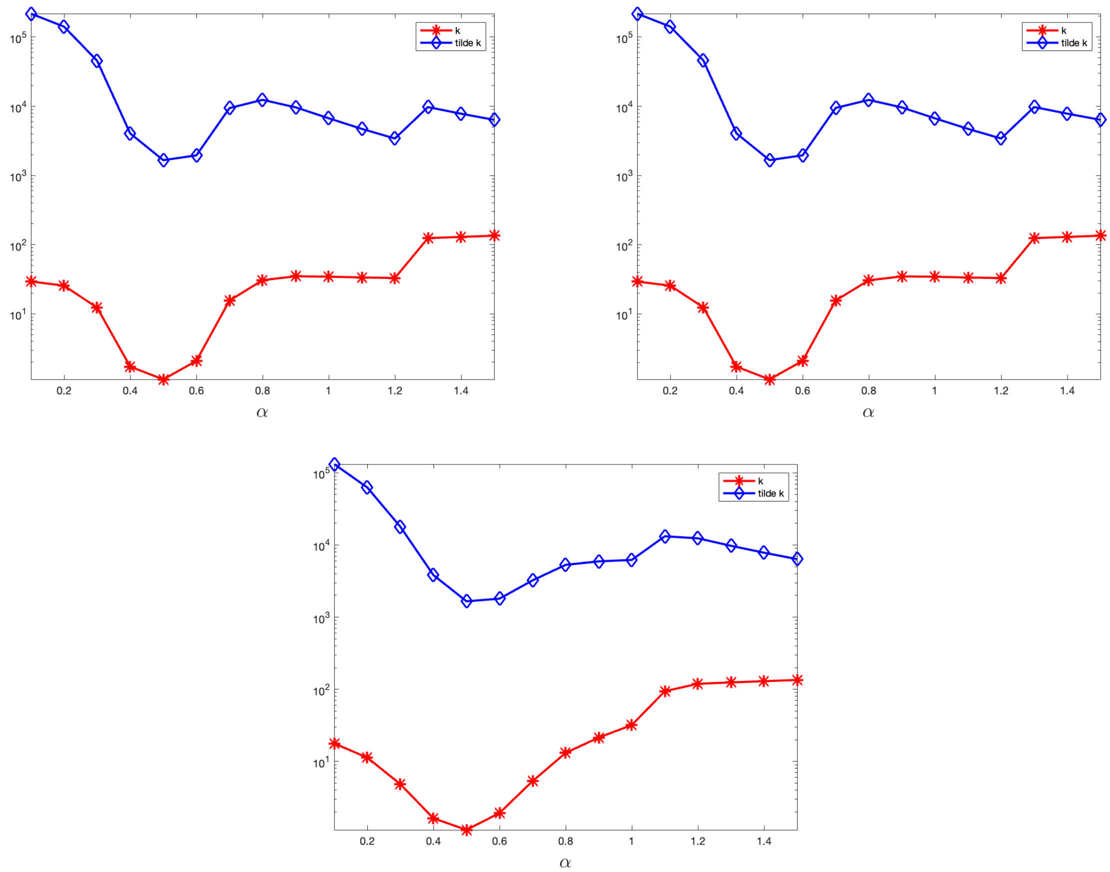

Figure 3: Test function $f_1(x) = e^{\frac{x}{2}} + \frac{x}{2}e^{-2x}$. The estimate $\tilde{\kappa}_{\alpha,\lambda}$ (blue '$\diamond$') and $\kappa_{\alpha,\lambda}$ (red '*') for different α values; $\sigma = 0$ (top,left), $\sigma = 1.0e-4$ (top,right), and $\sigma = 1.0e-2$ (bottom).

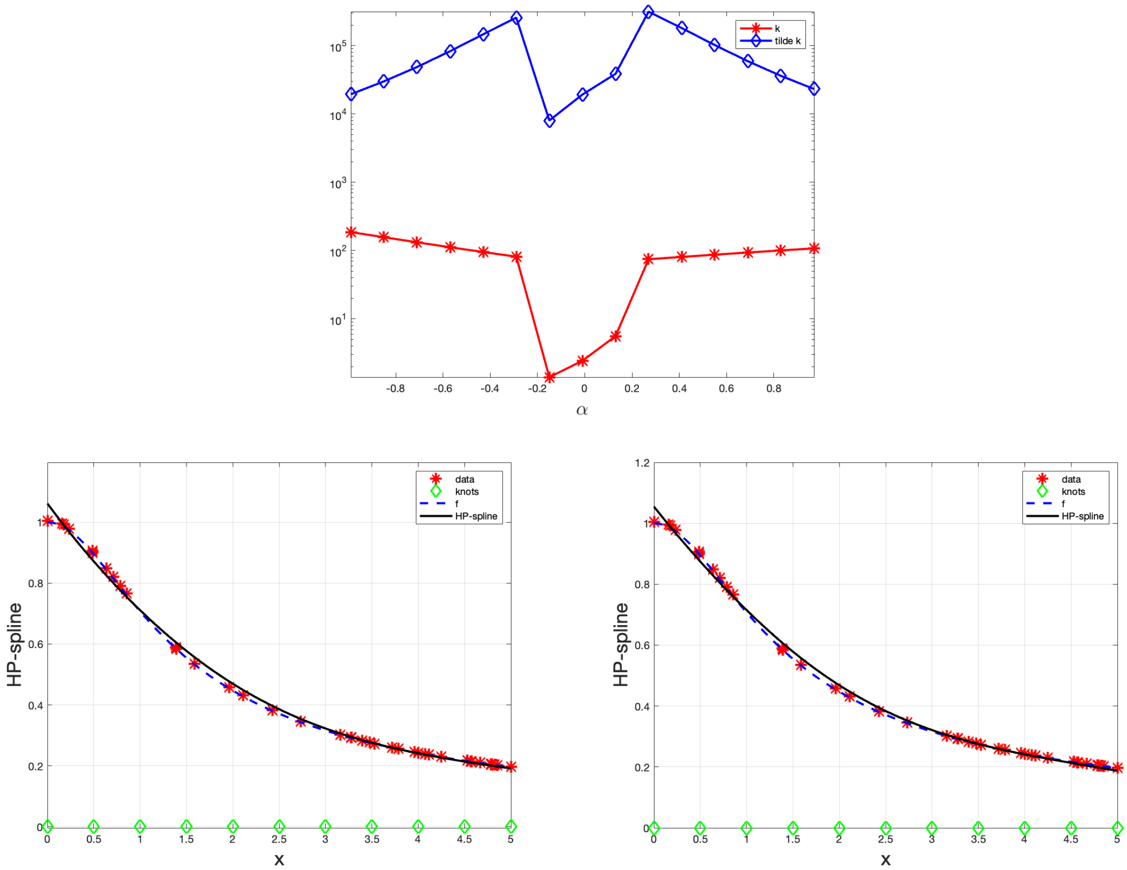

Figure 4: Test function f_2, with $\sigma = 1.0e-2$. From left to right: the estimate $\tilde{\kappa}_{\alpha,\lambda}$ (blue '$\diamond$') and $\kappa_{\alpha,\lambda}$ (red '*') for different values of α. (top). The HP-spline fitting the data $(x_i, \tilde{y}_i)_{i=1,\ldots,m}, \tilde{y}_i = f_2(x_i) + \sigma_i$, $m = 40$, with α minimizing $\kappa_{\alpha,\lambda}$ (bottom,left) and $\tilde{\kappa}_{\alpha,\lambda}$ (bottom,right).

The numerical results concerning f_2 are reported in Table 3; the ones for f_3 are in Table 4. All tables and graphs confirm the effectiveness of Algorithm 1 and Algorithm 2 to select the *optimal* frequency parameter α.

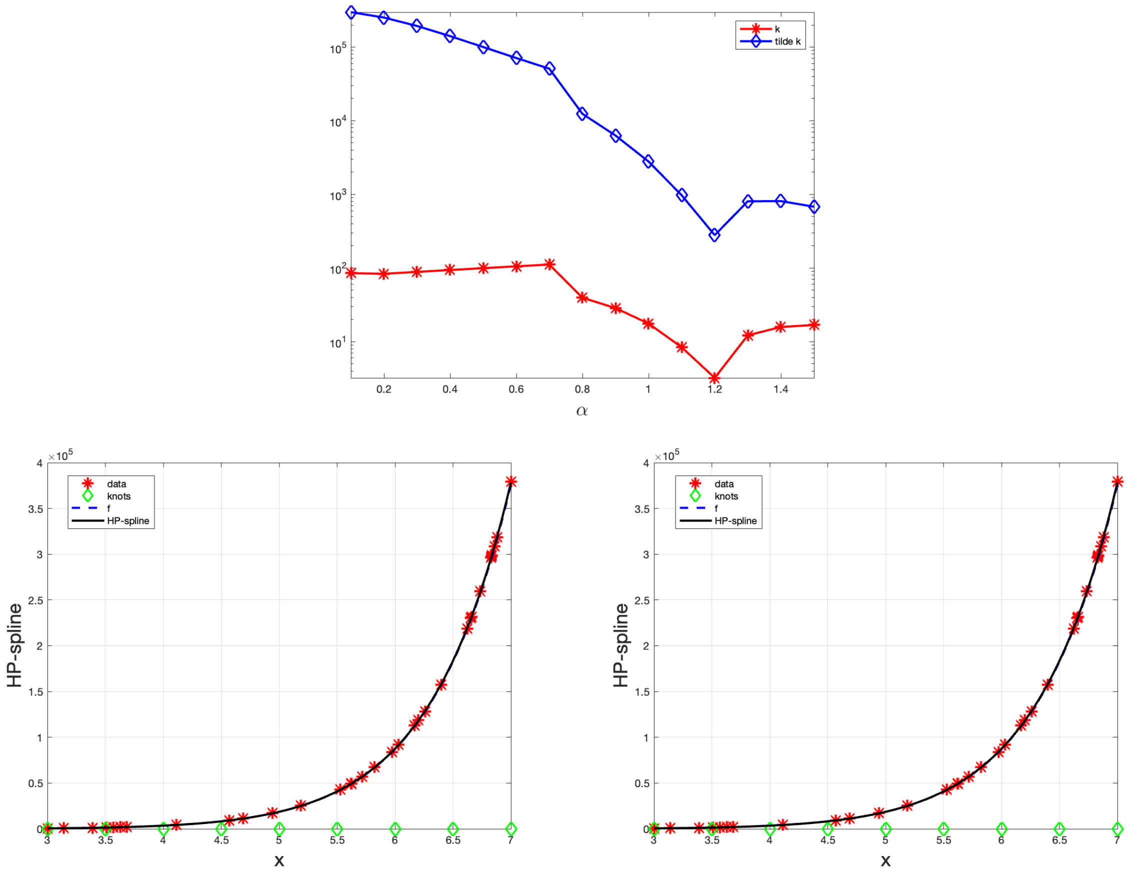

Figure 5: Test function f_3, with $\sigma = 1.0e-2$. From left to right: the estimate $\tilde{\kappa}_{\alpha,\lambda}$ (blue '$\diamond$') and $\kappa_{\alpha,\lambda}$ (red '*') for different values of α. (top). The HP-spline fitting the data $(x_i, \tilde{y}_i)_{i=1,\ldots,m}, \tilde{y}_i = f_3(x_i) + \sigma_i$, $m = 33$, with α minimizing $\kappa_{\alpha,\lambda}$ (bottom,left) and $\tilde{\kappa}_{\alpha,\lambda}$ (bottom,right).

$f_1(x) = e^{x/2} + 0.5x\ e^{-2x}$, $\alpha \in [0.1, 1.5]$					
α	λ	$\kappa_{\alpha,\lambda}$	$\tilde{\kappa}_{\alpha,\lambda}$	$\delta_{\alpha,\lambda}$	$\varepsilon_{\alpha,\lambda}$
$\sigma = 0$					
1.0000e-01	1.1733e-01	2.9412e+01	2.1835e+05	6.4104e-04	5.7663e-04
2.0000e-01	1.4614e-01	2.5611e+01	1.4163e+05	5.8838e-04	5.3080e-04
3.0000e-01	3.2889e-01	1.2332e+01	4.5566e+04	8.5160e-04	8.6482e-04
4.0000e-01	2.5373e+00	1.7304e+00	4.0569e+03	2.0365e-03	2.1499e-03
5.0000e-01	4.1912e+00	**1.1327e+00**	**1.6655e+03**	2.1897e-03	2.4445e-03
6.0000e-01	2.4472e+00	2.0947e+00	1.9539e+03	1.9731e-03	2.0808e-03
7.0000e-01	3.5473e-01	1.5582e+01	9.4283e+03	8.6364e-04	8.6258e-04
8.0000e-01	1.9347e-01	3.0756e+01	1.2401e+04	6.7100e-04	6.1147e-04
9.0000e-01	1.8276e-01	3.4992e+01	9.6651e+03	7.5519e-04	6.8688e-04
1.0000e+00	1.9864e-01	3.4542e+01	6.7137e+03	9.8927e-04	8.9734e-04
1.1000e+00	2.1835e-01	3.3652e+01	4.7205e+03	1.3390e-03	1.2137e-03
1.2000e+00	2.3760e-01	3.3057e+01	3.4261e+03	1.7869e-03	1.6238e-03
1.3000e+00	6.7243e-02	1.2461e+02	9.7511e+03	4.8025e-04	5.1426e-04
1.4000e+00	6.8767e-02	1.2975e+02	7.8193e+03	5.4119e-04	5.8577e-04
1.5000e+00	7.0319e-02	1.3485e+02	6.3742e+03	6.0501e-04	6.6568e-04
$\sigma = 10^{-4}$					
1.0000e-01	1.1777e-01	2.9301e+01	2.1753e+05	6.4948e-04	5.6477e-04
2.0000e-01	1.4667e-01	2.5518e+01	1.4112e+05	5.9476e-04	5.2398e-04
3.0000e-01	3.2609e-01	1.2438e+01	4.5957e+04	8.5012e-04	8.5752e-04
4.0000e-01	2.5371e+00	1.7306e+00	4.0573e+03	2.0387e-03	2.1517e-03
5.0000e-01	4.1876e+00	**1.1337e+00**	**1.6670e+03**	2.1899e-03	2.4466e-03
6.0000e-01	2.4476e+00	2.0944e+00	1.9535e+03	1.9753e-03	2.0818e-03
7.0000e-01	3.5252e-01	1.5680e+01	9.4874e+03	8.6310e-04	8.5608e-04
8.0000e-01	1.9539e-01	3.0454e+01	1.2279e+04	6.7884e-04	6.0687e-04
9.0000e-01	1.8418e-01	3.4723e+01	9.5907e+03	7.6419e-04	6.7650e-04
1.0000e+00	1.9962e-01	3.4372e+01	6.6808e+03	9.9885e-04	8.8256e-04
1.1000e+00	2.1901e-01	3.3551e+01	4.7065e+03	1.3486e-03	1.1957e-03
1.2000e+00	2.3806e-01	3.2993e+01	3.4195e+03	1.7964e-03	1.6038e-03
1.3000e+00	6.7243e-02	1.2461e+02	9.7511e+03	4.8236e-04	4.9632e-04
1.4000e+00	6.8767e-02	1.2975e+02	7.8193e+03	5.4321e-04	5.6697e-04
1.5000e+00	7.0319e-02	1.3485e+02	6.3742e+03	6.0694e-04	6.4649e-04
$\sigma = 10^{-2}$					
1.0000e-01	1.9423e-01	1.7767e+01	1.3190e+05	2.9078e-03	5.0101e-03
2.0000e-01	3.3073e-01	1.1317e+01	6.2584e+04	2.9001e-03	5.0782e-03
3.0000e-01	8.3745e-01	4.8432e+00	1.7895e+04	3.0665e-03	5.1964e-03
4.0000e-01	2.6902e+00	1.6321e+00	3.8264e+03	3.4166e-03	5.3326e-03
5.0000e-01	4.2111e+00	**1.1273e+00**	**1.6577e+03**	3.4923e-03	5.4628e-03
6.0000e-01	2.6525e+00	1.9326e+00	1.8026e+03	3.3758e-03	5.2677e-03
7.0000e-01	1.0340e+00	5.3455e+00	3.2345e+03	3.1177e-03	5.1477e-03
8.0000e-01	4.5241e-01	1.3153e+01	5.3032e+03	2.9556e-03	5.0193e-03
9.0000e-01	2.9798e-01	2.1463e+01	5.9281e+03	2.9643e-03	4.9353e-03
1.0000e+00	2.1486e-01	3.1935e+01	6.2070e+03	2.9701e-03	4.8820e-03
1.1000e+00	7.8076e-02	9.4113e+01	1.3202e+04	2.6655e-03	5.0772e-03
1.2000e+00	6.5799e-02	1.1937e+02	1.2372e+04	2.6464e-03	5.1029e-03
1.3000e+00	6.7296e-02	1.2451e+02	9.7434e+03	2.6624e-03	5.0799e-03
1.4000e+00	6.8820e-02	1.2965e+02	7.8133e+03	2.6816e-03	5.0571e-03
1.5000e+00	7.0373e-02	1.3475e+02	6.3693e+03	2.7042e-03	5.0355e-03

Table 2: Test function $f_1(x) = e^{x/2} + 0.5x\ e^{-2x}$: numerical results for different α values; from top to bottom we set $\sigma = 0$, $\sigma = 1.0e-4$ and $\sigma = 1.0e-2$.

$f_2(x) = 1/\sqrt{1+x^2}$, $\alpha \in [-0.9, 0.9]$					
α	λ	$\kappa_{\alpha,\lambda}$	$\tilde{\kappa}_{\alpha,\lambda}$	$\delta_{\alpha,\lambda}$	$\varepsilon_{\alpha,\lambda}$
-9.9000e-01	2.6228e-02	1.8639e+02	1.9411e+04	3.0208e-03	4.5103e-03
-8.5000e-01	2.9263e-02	1.5672e+02	2.9972e+04	3.0761e-03	4.4949e-03
-7.1000e-01	3.2684e-02	1.3217e+02	4.8609e+04	3.1731e-03	4.4957e-03
-5.7000e-01	3.6493e-02	1.1195e+02	8.2849e+04	3.3053e-03	4.5120e-03
-4.3000e-01	4.0728e-02	9.5238e+01	1.4633e+05	3.4607e-03	4.5408e-03
-2.9000e-01	4.5384e-02	8.1457e+01	2.5601e+05	3.6220e-03	4.5766e-03
$\boxed{\textbf{-1.5000e-01}}$	2.5174e+00	$\boxed{\textbf{1.4048e+00}}$	$\boxed{\textbf{8.0131e+03}}$	2.4701e-02	2.5885e-02
-1.0000e-02	1.3892e+00	2.4439e+00	1.9197e+04	1.8565e-02	1.9495e-02
1.3000e-01	6.3270e-01	5.5892e+00	3.8564e+04	1.2163e-02	1.2558e-02
2.7000e-01	5.2990e-02	7.4726e+01	3.1404e+05	3.6165e-03	4.5960e-03
4.1000e-01	5.4805e-02	8.0746e+01	1.8068e+05	3.5410e-03	4.5774e-03
5.5000e-01	5.6657e-02	8.7085e+01	1.0175e+05	3.4503e-03	4.5538e-03
6.9000e-01	5.8547e-02	9.3706e+01	5.9139e+04	3.3527e-03	4.5282e-03
8.3000e-01	6.0478e-02	1.0056e+02	3.6091e+04	3.2571e-03	4.5037e-03
9.7000e-01	6.2453e-02	1.0759e+02	2.3174e+04	3.1725e-03	4.4833e-03

Table 3: Test function $f_2(x) = 1/\sqrt{1+x^2}$, with $\sigma = 1.0e-2$: numerical results for different α values.

$f_3(x) = log(x^2) + x^3 e^x$, $\alpha \in [0.1, 1.5]$					
α	λ	$\kappa_{\alpha,\lambda}$	$\tilde{\kappa}_{\alpha,\lambda}$	$\delta_{\alpha,\lambda}$	$\varepsilon_{\alpha,\lambda}$
1.0000e-01	4.3249e-02	8.5260e+01	2.9875e+05	4.1794e-03	5.1683e-03
2.0000e-01	4.4171e-02	8.3616e+01	2.5211e+05	3.8616e-03	5.0866e-03
3.0000e-01	4.5108e-02	8.8724e+01	1.9384e+05	3.6276e-03	5.0692e-03
4.0000e-01	4.6058e-02	9.4084e+01	1.4110e+05	3.4628e-03	5.0927e-03
5.0000e-01	4.7024e-02	9.9688e+01	1.0031e+05	3.3518e-03	5.1385e-03
6.0000e-01	4.7971e-02	1.0560e+02	7.1171e+04	3.2801e-03	5.1932e-03
7.0000e-01	4.8969e-02	1.1166e+02	5.0941e+04	3.2360e-03	5.2473e-03
8.0000e-01	1.4902e-01	3.9553e+01	1.2426e+04	3.5008e-03	5.0095e-03
9.0000e-01	2.2203e-01	2.8577e+01	6.3082e+03	3.4675e-03	5.0119e-03
1.0000e+00	3.8660e-01	1.7640e+01	2.7941e+03	3.4563e-03	5.0597e-03
1.1000e+00	8.7130e-01	8.3996e+00	9.7468e+02	3.4451e-03	5.1836e-03
$\boxed{\textbf{1.2000e+00}}$	2.4298e+00	$\boxed{\textbf{3.2270e+00}}$	$\boxed{\textbf{2.7986e+02}}$	3.2390e-03	5.2544e-03
1.3000e+00	6.8671e-01	1.2212e+01	8.0661e+02	3.1857e-03	5.4052e-03
1.4000e+00	5.6491e-01	1.5849e+01	8.1158e+02	3.1864e-03	5.4648e-03
1.5000e+00	5.6564e-01	1.6869e+01	6.8088e+02	3.1853e-03	5.4625e-03

Table 4: Test function $f_3(x) = log(x^2) + x^3 e^x$, with $\sigma = 1.0e-2$: numerical results for different α values.

5.3. Test f_4

The last test concerns the function $f_4(x) = sin(x)cos(2x)$ in $[-3, 3]$ and it is given to compare the proposed criteria for selecting α based on the minimization of $\kappa_{\alpha,\lambda}$ and $\tilde{\kappa}_{\alpha,\lambda}$, with another possible strategy used by the authors in [11, 14]. There, the optimal α, say α_{opt}, was chosen by a nonlinear least-squares regression of the data using the 3-parameter function $r(\mathbf{c}, x) = c_1 e^{c_3 x} + c_2 e^{-c_3 x}$ belonging to the space $\mathbb{E}_{4,\alpha}$ with sign coherently set as $\alpha_{opt} = |c_3| sign(y_m - y_1)$. This fitting is computed by the MATLAB function `nlinfit`. Table 5 refers the α-values obtained by the three approaches with $n = 13$ knots uniformly distributed in $[a, b] = [-3, 3]$ with spacing $h = 0.5$, $m = 47$ data points and $\sigma = 0$. Fig. 6 shows the estimate $\tilde{\kappa}_{\alpha,\lambda}$ and $\kappa_{\alpha,\lambda}$ for different values of $\alpha \in [0.1, 1.5]$ (top,left). In the same figure, the approximation given by the HP-spline defined using α_{opt} (top, right) is comparable with the one defined using the α minimizing $\kappa_{\alpha,\lambda}$ (bottom, left); the α minimizing $\tilde{\kappa}_{\alpha,\lambda}$ gives a better approximation (bottom,right). The results are confirmed by the relative errors in the last column of Table 5.

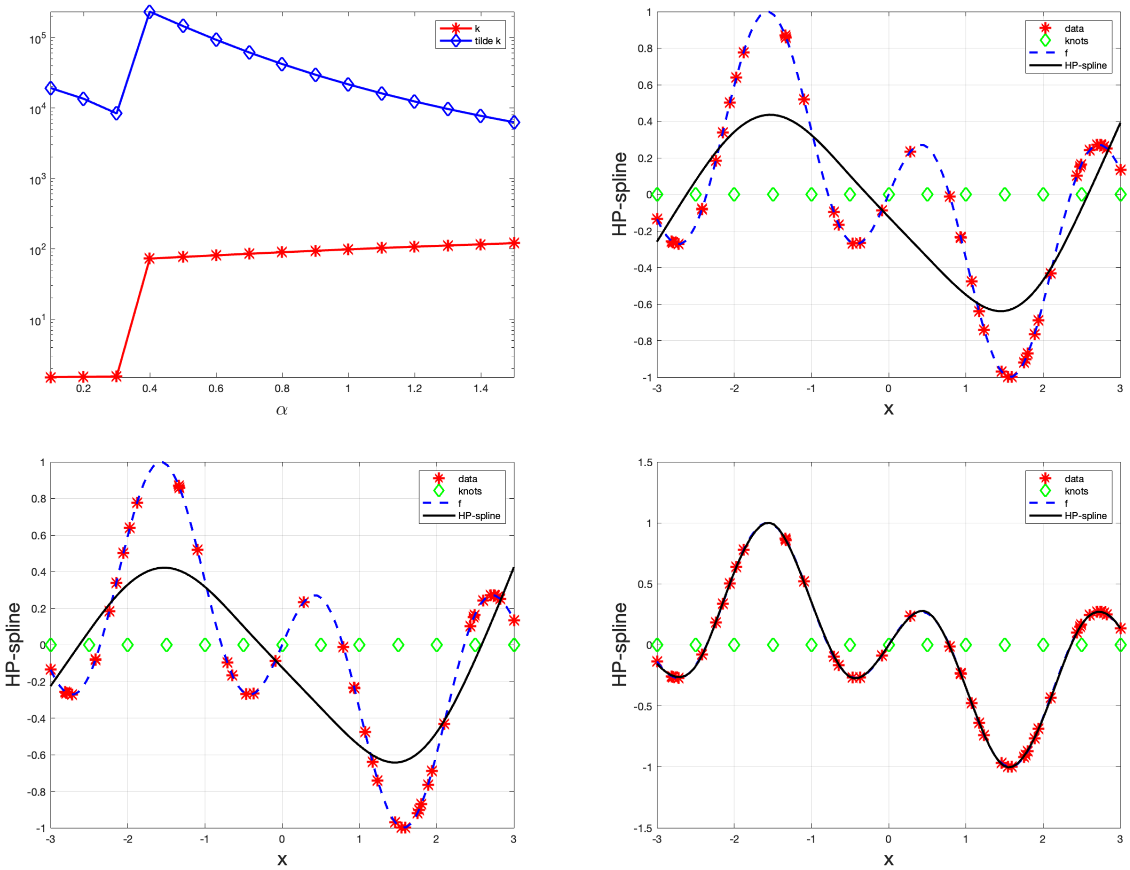

Figure 6: Test function f_4, with $\sigma = 0$. From left to right, top to bottom: the estimate $\tilde{\kappa}_{\alpha,\lambda}$ (blue '$\diamond$') and $\kappa_{\alpha,\lambda}$ (red '*') for different values of α (top,left). The approximation of f_4 by the HP-spline defined using α_{opt} (top,right), the HP-spline using α minimizing $\kappa_{\alpha,\lambda}$ (bottom,left) and the HP-spline using α minimizing $\tilde{\kappa}_{\alpha,\lambda}$ (bottom,right).

The numerical results concerning f_4 are in Table 5.

5.4. Test f_5

In this test we want to prove that the approximation by HP-spline has numerical issues when α approaches 0; this motivates the introduction of a threshold $\tau = 1.0e-5$, that bounds the minimum absolute value for the frequency parameter around the zero. We consider $f_5(x) = 1/(x - 11)$ and the following problem

$f_4(x) = sin(x)cos(2x), \quad \alpha \in [0.1, 1.5]$					
α	λ	$\kappa_{\alpha,\lambda}$	$\tilde{\kappa}_{\alpha,\lambda}$	$\delta_{\alpha,\lambda}$	$\varepsilon_{\alpha,\lambda}$
$\boxed{\mathbf{1.0000e-01}}$	2.3867e+00	$\boxed{\mathbf{1.5090e+00}}$	$\boxed{\mathbf{1.9249e+04}}$	5.0719e-01	6.1739e-01
2.0000e-01	2.5588e+00	1.5283e+00	1.3523e+04	5.1202e-01	6.2436e-01
3.0000e-01	2.7567e+00	1.5384e+00	8.3748e+03	5.1895e-01	6.3302e-01
4.0000e-01	6.3141e-02	7.2729e+01	2.3335e+05	9.0578e-03	9.8609e-03
5.0000e-01	6.4642e-02	7.6796e+01	1.4571e+05	9.0841e-03	9.8385e-03
6.0000e-01	6.6207e-02	8.0905e+01	9.3135e+04	9.1675e-03	9.8774e-03
7.0000e-01	6.7718e-02	8.5184e+01	6.1549e+04	9.2849e-03	9.9568e-03
8.0000e-01	6.9236e-02	8.9536e+01	4.2078e+04	9.4385e-03	1.0083e-02
9.0000e-01	7.0765e-02	9.3941e+01	2.9715e+04	9.6235e-03	1.0254e-02
1.0000e+00	7.2306e-02	9.8378e+01	2.1620e+04	9.8356e-03	1.0467e-02
1.1000e+00	7.3861e-02	1.0283e+02	1.6161e+04	1.0072e-02	1.0724e-02
1.2000e+00	7.5432e-02	1.0727e+02	1.2377e+04	1.0332e-02	1.1023e-02
1.3000e+00	7.7021e-02	1.1169e+02	9.6878e+03	1.0613e-02	1.1365e-02
1.4000e+00	7.8630e-02	1.1608e+02	7.7326e+03	1.0917e-02	1.1753e-02
$\boxed{\mathbf{1.5000e+00}}$	8.0261e-02	$\boxed{\mathbf{1.2043e+02}}$	$\boxed{\mathbf{6.2816e+03}}$	1.1244e-02	1.2189e-02
α_{opt}	λ	$\kappa_{\alpha_{opt},\lambda}$	$\tilde{\kappa}_{\alpha_{opt},\lambda}$	$\delta_{\alpha_{opt},\lambda}$	$\varepsilon_{\alpha_{opt},\lambda}$
2.0764e-03	2.2353e+00	1.5088e+00	2.2174e+04	5.0425e-01	6.1188e-01

Table 5: Test function $f_4(x) = sin(x)cos(2x)$, with $\sigma = 0$: numerical results for different α values (top) and for α_{opt} (bottom).

setting: $n = 21$ splines knots uniformly distributed in $[0, 10]$, spacing $h = 0.5$ and $m = 77$ data points. The numerical results, reported in Fig. 7, numerically show that indeed, there is a limit value for α, under which the algorithm doesn't work. Nevertheless, since from Figure 7 (bottom, right) we see that the P-spline has a reasonable behaviour, is it evident that this issue is not in the method but in the evaluation strategies. Indeed, the analytical expressions of the HB-splines in Appendix A are numerically unstable, and not reliable for practical implementations, for small (or large) values of $|\alpha|$. This is certainly another point to be further investigated.

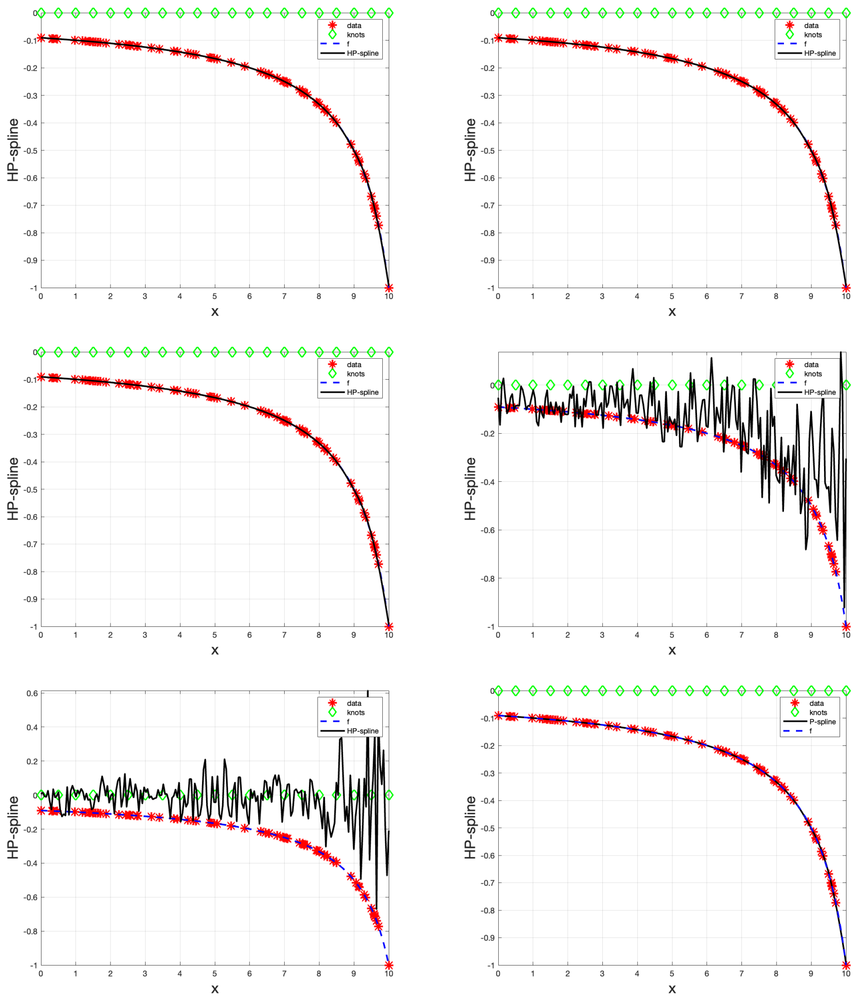

Figure 7: Test function $f_5(x) = 1/(x-11)$. The HP-spline (black '$-$') for $\alpha = 10^{-p}$, $p = 2, \ldots, 6$ and the P-spline for $\alpha = 0$ (reading by rows, from top left to bottom right).

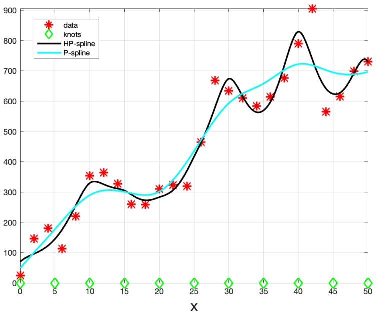

Figure 8: Test 6. The HP-spline (black '−') vs P-spline (cyan '−') on the increasing dataset in [23], set $n = 11$ and $\alpha = 0.4$.

5.5. Test 6

The last test is to investigate the action of HP-splines when dealing with experimental data corresponding to coal production in Nigeria, from 1916 to 2001. This data set is taken from [23] where a comparison of linear and exponential regression is presented. For one of the datasets in [23], we show that HP-spline captures the data behavior better than the standard P-spline fitting. Table 6 reports the relative root mean square errors obtained by our HP-spline and the P-spline, for the $m = 15$ historical values and for different number of knots n and $\alpha = 0.4$. Figure 8 shows the graphs of both the HP-spline and the P-spline for the case $n = 11$.

n	HP-spline	P-spline
7	3.6248e-02	3.5421e-02
8	3.4430e-02	3.5122e-02
11	2.7693e-02	3.0535e-02
12	1.7359e-02	2.8186e-02
18	1.4915e-02	2.2460e-02
20	4.4294e-03	1.2874e-02

Table 6: Relative root mean square errors

6. Conclusions

This paper discusses a linear algebra-based methodology for the frequency parameter selection of hyperbolic - polynomial P-splines (HP-splines) that are penalized splines with segments in an exponential - polynomial space. Indeed, the HP-spline model requires an effective strategy to select the frequency parameter in addition to the one needed for the smoothing parameter. Here, we propose a computational method that involves a linear algebra procedure for the Tikhonov regularization problem adapted to the HP-splines context. As shown in the numerical experiments, this technique provides an efficient data-driven parameter selection strategy corresponding to HP-splines that better capture the trend suggested by the fitted data. Automatic frequency detection, in our opinion, is crucial to infer information hidden in the input data. We conclude by mentioning that the analysis of the HP-spline model is not jet completed: the selection of the B-spline knots, the interrelation knots-data and the lack of symmetry of the proposed penalty are critical aspects that we plan to study in the near future.

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Appendix A. Computation of HB-splines

In [13] HB-splines have been defined with pieces expressed in terms of proper Bernstein(-like) local bases and for any type of knots distribution. Here, we follow the approach described in [15] for the cardinal setting where HB-splines are defined through convolution. With 'cardinal' setting we mean that the spline knots are *integers and equidistant, with constant separation* $h = 1$.

Given the set of frequencies $\alpha_1, \cdots, \alpha_\ell$, starting from the first order cardinal HB-spline $b^1_{\alpha_1}$ (where the superscript 1 is to recall the knots distance) defined as

$$b^1_{\alpha_1}(x) = e^{\alpha_1 x}\chi_{[0,1]}(x), \tag{A.1}$$

the HB-spline of order ℓ is obtained by successive convolution of ℓ HB-splines of order one

$$b^1_{\alpha_1,\alpha_2\cdots,\alpha_\ell}(x) = \left(b^1_{\alpha_1} * b^1_{\alpha_2} \cdots * b^1_{\alpha_\ell}\right)(x).$$

Figure A.9 shows the graph of the cardinal HB-splines of order from 1 to 4 corresponding to the choice $\alpha_1 = 1$, $\alpha_2 = -1$, $\alpha_3 = 0$, $\alpha_4 = 0$.

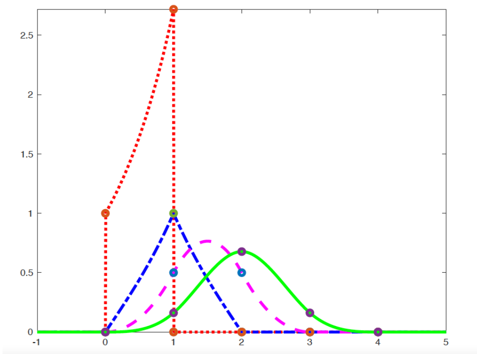

Figure A.9: The cardinal HB-splines b^1_1, $b^1_{1,-1}$, $b^1_{1,-1,0}$ and $b^1_{1,-1,0,0}$ obtained via convolution.

Below, we provide the explicit piecewise-defined expression of the cardinal HB-spline of order 4, $b^1_{\boldsymbol{\alpha}}$, supported on $[0,4]$ where we use the short hand notation $\boldsymbol{\alpha} = (\alpha, \alpha, -\alpha, -\alpha)$.

Proposition Appendix A.1. *The CHB-spline* $b^1_{\boldsymbol{\alpha}}$ *with support* $[0,4]$ *is:*

$$b^1_{\boldsymbol{\alpha}}(t) = \begin{cases} \left(t2\cosh(\alpha t) - \frac{1}{\alpha}2\sinh(\alpha t)\right)/4\alpha^2 & t \in (0,1] \\ \left(-2(t-1)2\cosh(\alpha(t-2)) - (t-2)2\cosh(\alpha t) + \frac{2}{\alpha}2\sinh(\alpha(t-2)) + \frac{1}{\alpha}2\sinh(\alpha t)\right)/4\alpha^2 & t \in (1,2] \\ \left((t-2)2\cosh(\alpha(t-4)) + 2(t-3)2\cosh(\alpha(t-2)) - \frac{1}{\alpha}2\sinh(\alpha(t-4)) - \frac{2}{\alpha}2\sinh(\alpha(t-2))\right)/4\alpha^2 & t \in (2,3] \\ \left((4-t)2\cosh(\alpha(t-4)) + \frac{1}{\alpha}2\sinh(\alpha(t-4))\right)/4\alpha^2 & t \in (3,4] \end{cases} \tag{A.2}$$

Proof. From (A.1), recalling that $(g*g)(t) = \int_{-\infty}^{\infty} g(s)g(t-s)ds$ it is simple to get the expression of the HB-spline $b^1_{\alpha,-\alpha}$ and use it to make another round of convolution. Indeed, fo

$$g(t) = b_{\alpha,-\alpha}(t) = \begin{cases} g_1(t) = \frac{e^{\alpha t} - e^{-\alpha t}}{2\alpha} & t \in (0,1] \\ g_2(t) = \frac{e^{\alpha(2-t)} - e^{-\alpha(2-t)}}{2\alpha} & t \in (1,2] \\ 0 & \textit{otherwise} \end{cases} \tag{A.3}$$

we compute

$$(g*g)(t) = \int_0^1 g_1(s)g(t-s)ds + \int_1^2 g_2(s)g(t-s)ds \tag{A.4}$$

by expressing, via the variable change $t = s - \tau$, the two integrals as

$$\int_{t-1}^{t} g_1(t-\tau)g(\tau)d\tau \quad \text{and} \quad \int_{t-2}^{t-1} g_2(t-\tau)g(\tau)d\tau.$$

To get that the value of $\int_{t-1}^{t} g_1(t-\tau)g(\tau)d\tau$ we need to specialize the variation of t providing:

$$\begin{cases} 0 & if\ t \le 0 \\ \int_0^t g_1(t-\tau)g_1(\tau)d\tau & if\ t \in (0,1] \\ \int_{t-1}^1 g_1(t-\tau)g_1(\tau)d\tau + \int_1^t g_1(t-\tau)g_2(\tau)d\tau & if\ t \in (1,2] \\ \int_{t-1}^2 g_1(t-\tau)g_2(\tau)d\tau & if\ t \in (2,3] \\ 0 & if\ t > 3 \end{cases}$$

and similarly, for the computation of $\int_{t-2}^{t-1} g_2(t-\tau)g(\tau)d\tau$ that is

$$\begin{cases} 0 & if\ t \le 1 \\ \int_0^{t-1} g_2(t-\tau)g_1(\tau)d\tau & if\ t \in (1,2] \\ \int_{t-2}^1 g_2(t-\tau)g_1(\tau)d\tau + \int_1^{t-1} g_2(t-\tau)g_2(\tau)d\tau & if\ t \in (2,3] \\ \int_{t-2}^2 g_2(t-\tau)g_2(\tau)d\tau & if\ t \in (3,4] \\ 0 & if\ t > 4 \end{cases}$$

Integrating on the corresponding intervals, the functions:

$$\begin{aligned} g_1(t-\tau)g_1(\tau) &= \left((e^{\alpha\, t} + e^{-\alpha\, t}) - (e^{\alpha\,(t-2\tau)} + e^{-\alpha\,(t-2\tau)})\right)/4\alpha^2, \\ g_1(t-\tau)g_2(\tau) &= \left(-(e^{\alpha\,(t-2)} + e^{-\alpha\,(t-2)}) + (e^{\alpha\,(t-2\tau+2)} + e^{-\alpha\,(t-2\tau+2)})\right)/4\alpha^2, \\ g_2(t-\tau)g_1(\tau) &= \left(-(e^{\alpha\,(2-t)} + e^{-\alpha\,(2-t)}) + (e^{\alpha\,(-t+2\tau+2)} + e^{-\alpha\,(-t+2\tau+2)})\right)/4\alpha^2, \\ g_2(t-\tau)g_2(\tau) &= \left((e^{\alpha\,(4-t)} + e^{-\alpha\,(4-t)}) - (e^{\alpha\,(-t+2\tau)} + e^{-\alpha\,(-t+2\tau)})\right)/4\alpha^2, \end{aligned}$$

we see that, the CHB-spline $b^1_{\boldsymbol{\alpha}}$ is piecewise defined as in (A.2). □

Using Proposition Appendix A.1, the CHB-splines supported in $[k, k+4]$ is obtained by suitable shift, for any $k \in \mathbb{N}$. In case the knots are uniform but with a distance $h \neq 1$, with the change of variable $x \to x/h$ we can work with the dilated version $B^h_{\boldsymbol{\alpha}h} := b^1_{\boldsymbol{\alpha}h}(\frac{\cdot}{h})$.

With all these preliminaries, we are now ready to define the HB-basis associated to a set of data points and based on a prescribed number of knots n.

Definition Appendix A.1. Let the data points $(x_i, y_i),\ i = 1, \ldots, m,\ x_1 < \cdots < x_m$, be given together with the uniform knots partition $\Xi := \{x_1 := a = \xi_1 < \xi_2 \cdots < \xi_n = b =: x_m\}$ $(n < m)$ extended with the uniform left and right extra knots $\xi_\ell = \xi_1 + (\ell-1)h,\ \ell = -2, -1, 0,\ \xi_{n+\ell} = \xi_n + \ell h,\ \ell = 1, 2, 3$ where $h = (b-a)/(n-1)$. The spline basis $\{B^\alpha_0, \ldots, B^\alpha_{n+1}\}$ with segments in $\mathbb{E}_{4,\alpha}$ consists of the uniform HB-splines $B^\alpha_0 := B^h_{\boldsymbol{\alpha}h}(\cdot - \xi_{-2})$ and its translates $B^\alpha_j = B^\alpha_0(\cdot - jh),\ j = 1, \cdots, n+1$.

Remark Appendix A.2. The (cardinal) B-splines are constructed by using knot $\xi_{-2},\ \xi_{-1},\ \xi_0,\ \xi_{n+1},\ \xi_{xn+2},\ \xi_{-n+3}$ outside the data interval $[x_1, x_m]$. Though the use of open-knot sequence could be more appropriate (see [22]) and recommended, we consider knots outside the data interval. The use of extreme knots is something to be investigated since it is connected with the so called 'boundary effects' of the model already mentioned by Eilers and Marx in their pioneering paper on P-splines [10].

Below we provide the explicit piecewise-defined expression of the HB-spline of order 4 on the uniformly distributed knots with distance h:

Proposition Appendix A.3. *The of order 4 HB-spline, 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 defined as*

$$\begin{cases} \left(\frac{t}{h}2\cosh(\alpha t) - \frac{1}{h\alpha}2\sinh(\alpha t)\right)/4(\alpha\, h)^2 & t \in (0, h] \\ \left(-4(\frac{t-h}{h})\cosh(\alpha(t-2h)) - \left(\frac{t-2h}{h}\right)2\cosh(\alpha t) + \frac{4}{h\alpha}\sinh(\alpha(t-2h)) + \frac{1}{h\alpha}2\sinh(\alpha t)\right)/4(\alpha\, h)^2 & t \in (h, 2h] \\ \left(\left(\frac{t-2h}{h}\right)2\cosh(\alpha(t-4h)) + 4\left(\frac{t-3h}{h}\right)\cosh(\alpha(t-2h)) - \frac{1}{h\alpha}2\sinh(\alpha(t-4h)) - \frac{4}{h\alpha}\sinh(\alpha(t-2h))\right)/4(\alpha\, h)^2 & t \in (2h, 3h] \\ \left(-(\frac{t-4h}{h})2\cosh(\alpha(t-4h)) + \frac{1}{h\alpha}2\sinh(\alpha(t-4h))\right)/4(\alpha\, h)^2 & t \in (3h, 4h] \end{cases} \tag{A.5}$$