SPLINE MODELS FOR DATA REPRESENTATION

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joint work with: **Salvatore Cuomo** and **Rosanna Campagna**

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What is a spline?

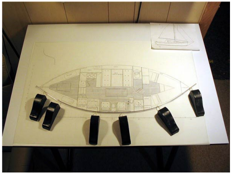
What is a spline?

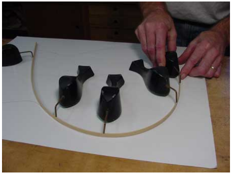
- A spline is a physical tool used by shipbuilders to draw ship profiles
- A spline is a piecewise-defined function with a certain regularity

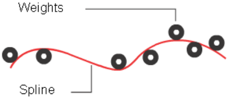
From ships to data analysis: a brief history of the spline

1. Originally developed for ship-building in the days before computer modeling, a spline is a *thin strip of wood pulled into place by weights called ducks or knots*. Naval architects use a spline to draw a smooth curve through a set of points via

2. The influence of each weight is greatest at the point of contact, and decreases smoothly further along the spline. *To get more control over a certain region of the spline, the draftman simply add more weights.*

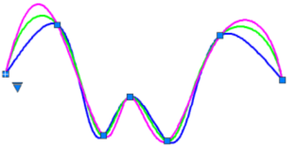


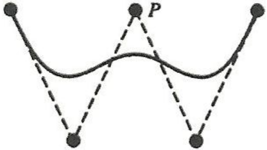




Splines for data analysis

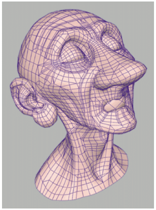
Mathematically a spline is a piecewise-defined function with a **prescribed** regularity at the 'conjuctions'

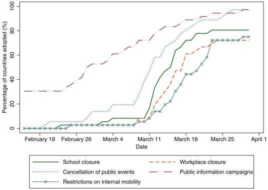


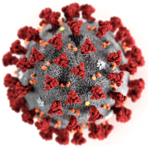


Where are they used?

Splines find application in several domains: animation or modeling

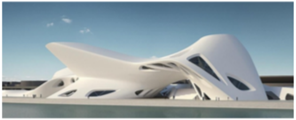


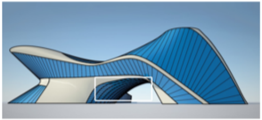


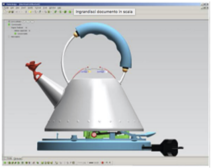


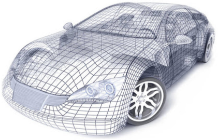
Where are they used?

Other domains of application are, Architecture, Design, Art, Automotive









Splines were introduced by
Isaac Jacob Schoenberg

Romanian-American mathematician (1903-1990)

SPLINE INTERPOLATION AND BEST QUADRATURE FORMULAE

BY I. J. SCHOENBERG

Communicated by Felix Browder, October 9, 1963

1. **The spline interpolation formula.** A spline function $S(x)$, of degree $k(\geqq 0)$, having the knots

$$x_0 < x_1 < \cdots < x_n, \tag{1}$$

is by definition a function of the class C^{k-1} which reduces to a polynomial of degree not exceeding k in each of the $n+2$ intervals in which the points (1) divide the real axis. The function $S(x)$ is seen to depend linearly on $n+k+1$ parameters. In [5, Theorem 2, p. 258] are given the precise conditions under which we can interpolate uniquely by $S(x)$ arbitrarily given ordinates at $n+k+1$ points on the real axis.

For the remainder of this note we set $k=2m-1$ $(1\leqq m\leqq n)$ and single out from this family of spline functions the

CLASS Σ_m: *The class of spline functions $S(x)$ of degree $2m-1$, knots (1), and the additional property that $S(x)$ reduces to polynomials of degree not exceeding $m-1$ in each of the ranges $(-\infty, x_0)$ and $(x_n, +\infty)$.*

The restriction that $m\leqq n$ is essential, otherwise Σ_m reduces to π_{m-1} (here and below π_k denotes a generic polynomial of degree $\leqq k$, as well as their class). In a paper [1] soon to appear C. de Boor ob-

JOURNAL OF APPROXIMATION THEORY 2, 167–206 (1969)

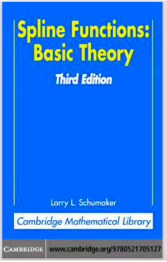
Cardinal Interpolation and Spline Functions*

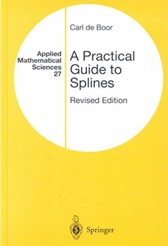
I. J. SCHOENBERG

Mathematics Research Center, U.S. Army, University of Wisconsin, Madison, Wisconsin

Splines a short history

A great impulse to splines was given by the work of
Larry Schumacker (Nashville, USA) and Carl de Boor (Madison, USA)





Since the work of I.J.Schoenberg

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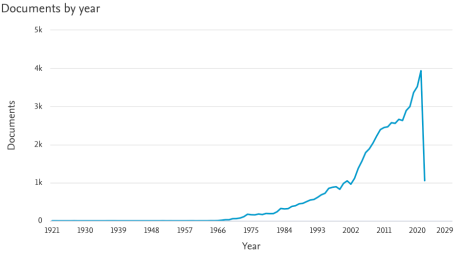


The Zoo of Splines

There is a large variety of spline species, referred to as the zoo of splines.

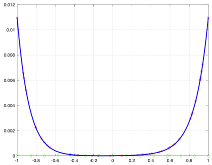
- Polynomial splines
- Exponential splines
- Rational splines
- Subdivision splines
- Chebyshev splines
- ...

They find application in many different contexts ranging from geometric modeling, image analysis, data approximation, solution of PDE...

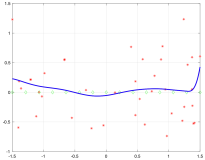
Interpolating, Smoothing, Approximating

My interest in splines is three-fold:

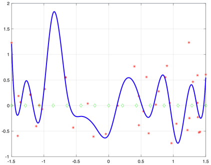
1. Interpolate exact data



2. Smooth noisy data



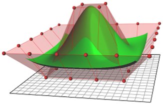
3. Approximate given data

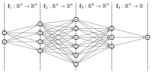


Spline models for data analysis and more

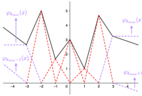
Spline models are also state-of-the-art technique **to infer knowledge from data**:

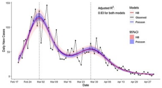
1. To model geometries in CAGD
2. As activation functions for Deep Learning
3. In data analysis, to predict data behaviour





$\mathbf{f}_{\text{deep}} = \mathbf{f}_4 \circ \mathbf{f}_3 \circ \mathbf{f}_2 \circ \mathbf{f}_1 : \mathbb{R}^2 \to \mathbb{R}$





Polynomial splines: Definition in the simplest case

Spline

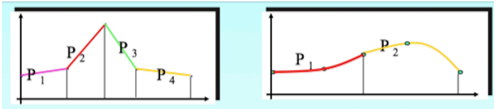
Given $[a,b]$, m knots $\Xi \equiv \{a=\xi_1 < \xi_2 < \ldots . < \xi_m = b\}$, a spline $s_{p,\Xi}$ of degree p (order $p+1$) and knots Ξ, is a **piecewise polynomial** such that:

$$s\big|_{[\xi_i,\xi_{i+1}]} \in \Pi_p, \quad i=1,\ldots,m-1,$$

$$s^{(j)}(\xi_i) = s^{(j)}(\xi_i), \quad i=2,\ldots,m-1, \quad j=0,..,p-1$$

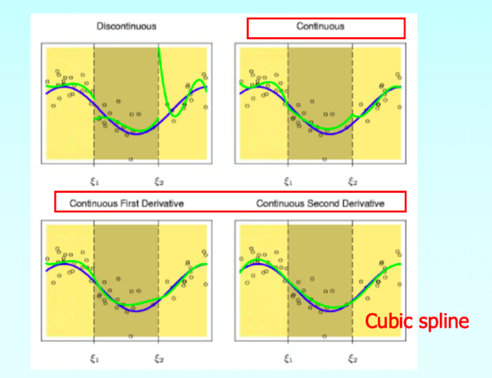
• A linear spline ($p=1$) is made of $m-1$ strait lines connected at the spline knots ξ_i, $i=1,\cdots,m$ in such a way that function is continuous in $[a,b]$;

• A quadratic splines ($p=2$) is made of $m-1$ parabola arcs connected at the spline knots ξ_i, $i=1,\cdots,m$ in such a way that function and first derivatives are continuous (no cups!) in $[a,b]$



Polynomial splines: examples

• A cubic spline ($p = 3$), is made of $m - 1$ cubic arcs in such a way that function, first and second derivatives are continuous in $[a, b]$.



Dimension of the spline space

How many degrees of freedom are needed to univocally identify a spline?

In the sub-intervals $I_1, \cdots, I_{m-1}$, a spline is a polynomial of degree p which means that it is given by giving $(p+1)$ coefficients. Hence, $S_{p,y}$ is given by $(m-1) \times (p+1)$ coefficients. At the 'internal' knots $\xi_2, \cdots, \xi_{m-1}$ all derivates up to order $p-1$ must agree, hence

$$\lim_{x \to \xi_i^-} S_{p,\Xi}^{(j)}(x) = \lim_{x \to \xi_i^+} S_{p,\Xi}^{(j)}(x), \quad \text{for } j = 0, \cdots, p-1, \quad (m-2) \times p \quad \text{conditions.}$$

Taking the difference, the number of free parameters of $S_{p,\Xi}$ are

$$(m-1) \times (p+1) - (m-2) \times p = m + p - 1.$$

Essentially, once p and the internal knots are given, a spline is identified by fixing $m + p - 1$ coefficients and $(m-2) + p + 1$ is the *dimension of the spline space*.

Beyond 'classical' polynomial splines

A similar definition and analysis of the spline space can be done in a more general context

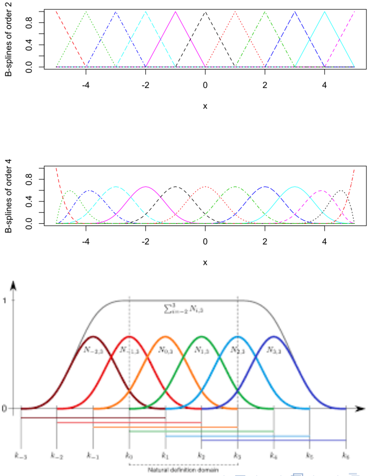
- different knots moltiplicities
- different degree for the segments
- different types of segments
- ...

B-spline bases of spline spaces

Relevant to our discussion: every spline space posses an **optimal** basis

B-splines:

1. are 'bell-shaped' ;
2. non-negative;
3. compactly supported;
4. partition of unity;



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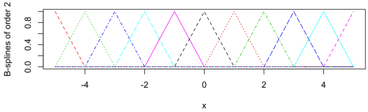

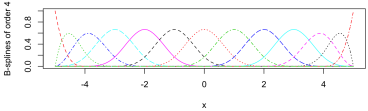

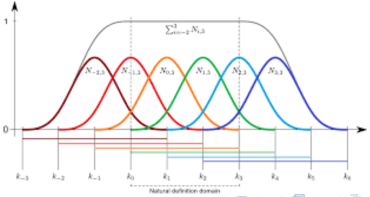

Splines in action for data analysis

Goal: to construct a good model for a given data set.

Definition (Least-squares polynomial spline)

Given the noisy data (x_i, y_i), $i = 1, \ldots, n$, a LS polynomial spline $s \in \mathcal{S}_p$ based on the knots $\xi_1 \cdots, \xi_m$, approximates the data set by minimizing the error with respect to the data

$$\underset{a_1,\cdots,a_{m+p-1}}{arg\ min} \sum_{i=1}^{n} w_i (y_i - s(x_i))^2, \qquad with \qquad s(x) = \sum_{j=1}^{m+p-1} a_j B_j(x)$$

☞ One needs to decide the number and the locations of the knots, $\xi_1, \ldots, \xi_m$, needed to define the B-spline basis functions B_j, $j = 1, \ldots, m+p-1$.

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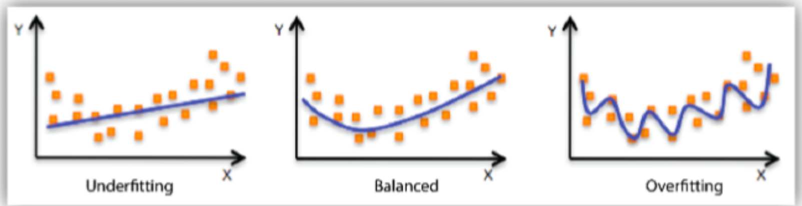
The correct model

☞ If the knots and the abscissa of data coincide the spline is interpolating that is when $s(x_i) = y_i, \; i = 1, \cdots, n$ (a problem if the data is noisy causing overfitting!).



Smoothing Spline

To prevent overfitting a penalty term can be introduced

Definition (Smoothing polynomial spline)

The smoothing spline is the solution of the **penalized least sq. problem**,

$$\underset{a_1,\dots,a_{n+p-1}}{\arg\min} \sum_{i=1}^{n} w_i(y_i - s(x_i))^2 + \lambda \int_a^b (s^{(p-1)})^2 dx, \quad \text{with} \quad s(x) = \sum_{j=1}^{n+p-1} a_j B_j(x)$$

where $x_1, \dots, x_n$ are set as the spline knots and the smoothing parameter λ affects the variability/fidelity with respect to the data.

☞ Drawback: selection of λ and the coincidence of knots/abscissa.... $\lambda = 0$ overfitting $\lambda >> 1$ underfitting

☞ CV, GCV, L-curves are the most used methods to select λ

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P-splines

In 1986 Eilers and Marx [1] propose a new family of splines with penalty:

P-splines ingredients

1. $\mathcal{S}_3$ **cubic spline** space spanned by **polynomial cubic B-splines**;
2. **uniform set of** m **knots** $\{\xi_1, \ldots, \xi_m\}$ (dimension of the space $m+2$);
3. $\sum_{j\in\mathbb{Z}} a_j B_j''(x) = \sum_{j\in\mathbb{Z}} (\Delta^2 \mathbf{a})_j b_j(x)$, where $(\Delta^2 \mathbf{a})_j = a_j - 2a_{j-1} + a_{j-2}$,
4. a certain level of **approximation**

[1] P. H. C. Eilers, B. D. Marx,(1996) Flexible smoothing with B-splines and penalties, Statistical Science 11.

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Penalized Splines

Definition (P-Spline)

Given n real data points $(x_i, y_i), i = 1, \dots, n$, $x_1 < \cdots < x_n$, and the **cubic spline space** $\mathcal{S}_3$ of dimension $m+2$ ($m-2$ internal knots), defined on $[a, b]$, with $a \le x_1$ and $x_n \le b$ spanned by $m+2$ polynomial cubic B-splines B_j, $j = 1, \dots, m+2$ based on the uniform set of knots $\{\xi_1, \dots, \xi_m\}$ with $\xi_1 \equiv a$ and $\xi_m \equiv b$.
The P-spline $s(x) = \sum_{j=1}^{m+2} a_j B_j(x)$, solve the penalized least squares problem

$$\min_{a_1,\dots,a_{m+2}} \sum_{i=1}^{n} w_i \left(y_i - \sum_{j=1}^{m+2} a_j B_j(x_i) \right)^2 + \lambda \sum_{j=3}^{m+2} \left((\Delta^2 \boldsymbol{a})_j \right)^2$$

with respect to the spline coefficients $\boldsymbol{a} = (a_1, \dots, a_n)$ while $(w_1, \dots, w_n)$ are weights and λ is a regularization parameter.

Pspline properties

The work of Eilers and Marx on P-splines has led to important developments in data regression through splines.

P-splines have a number of useful properties, inherited from B-splines:

- P-splines fit constant and linear polynomial data exactly;
- P-splines conserve moments (mean, variance) of the data;
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Beyond P-splines: a motivating application

Define **data-driven models** for **data analysis and forecasting** of **exponential data** is a frequent need in *nuclear magnetic resonance studies*, *atmospheric pressure changes*, *epidemic growth patterns*, etc.

Exponential data analysis

Given (x_i, y_i), $i = 1, \ldots, n$, a finite set of *noisy* data,

$$y_i = f(x_i) + \varepsilon_i, \quad i = 1, \ldots, n, \qquad \varepsilon_i \text{ unknown noise sources}$$

where f is *the weighted sum* of exponential functions

$$f(x) = \sum_{j=1}^{M} c_j e^{\alpha_j x}, \qquad \alpha_j \in \mathbb{R}.$$

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Beyond P-splines

Our plan:

- Replace polynomial splines $\Rightarrow$ with **exponential-polynomial splines**
- Extend polynomial B-splines $\Rightarrow$ **exponential-polynomial B-splines**
- Generalize the polynomial P-splines idea $\Rightarrow$ define **HP-splines**

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Beyond P-splines

We consider a two- and a four-dimensional exponential space for $\alpha \in \mathbb{R}$

$$\mathbb{E}_{2,\alpha} := \mathrm{span}\{e^{-\alpha x},\ x\, e^{-\alpha x}\}, \quad \mathbb{E}_{4,\alpha} := \mathrm{span}\{e^{\alpha x},\ x\, e^{\alpha x},\ e^{-\alpha x},\ x\, e^{-\alpha x}\}$$

that are the null spaces of suitable differential operators $\mathcal{L}_2$ and $\mathcal{L}_2^* \mathcal{L}_2$:

$$\mathcal{L}_2 u := u'' + 2\alpha\, u' + \alpha^2\, u, \quad \mathcal{L}_2^* \mathcal{L}_2 = v^{(iv)} - 2\alpha^2\, v'' + \alpha^4\, v, \qquad \alpha \in \mathbb{R}.$$

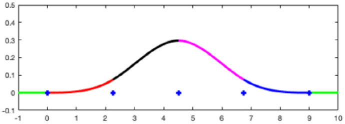
☞ We consider splines with segments in these spaces.

Beyond P-splines

We defined[2] an optimal basis for **hyperbolic-polynomial splines**:

HB-splines:

- with a bell-shaped graph;
- with a compact support identified by 5 uniform knots;
- C^2-regular, and with segments in the space $\mathbb{E}_{4,\alpha}$;
- reproducing functions in $\mathbb{E}_{2,\alpha}$.



Graph of an exponential-polynomial B^{α}-spline

[2] R. Campagna, C. Conti, S. Cuomo, Smoothing exponential-polynomial splines for multiexponential decay data, Dolomites Res. Notes Approx. 12 (2019) 86–100.

Beyond P-splines

To define a new family of hyperbolic-polynomial penalized splines (HP-splines), we start by considering the penalized least square problem

$$\min_{a_1,\ldots,a_{m+2}} \sum_{i=1}^{n} w_i \left(y_i - \sum_{j=1}^{m+2} a_j B_j^{\alpha}(x_i) \right)^2 + \lambda \int_a^b \left(\sum_{j=1}^{m+2} a_j \mathcal{L}_2 B_j^{\alpha}(x) \right)^2 dx.$$

Following the P-spline idea we substitute $\mathcal{L}_2$ with a **difference operator**:

$$\Delta_2^{h,\alpha} u = e^{\alpha h} u(x+h) - 2u(x) + e^{-\alpha h} u(x-h), \quad x \in [a,b], \quad \alpha, h \in \mathbb{R}$$

Approximation levels

- we use the uniformity of the knots, $B_j^\alpha(x-\ell h)=B_{j+\ell}^\alpha(x)$ and write:

$$\sum_{j=1}^{m+2} a_j \Delta_2^{h,\alpha} B_j^\alpha(x) = \sum_{j=1}^{m+2} a_j \left(e^{\alpha h} B_{j-1}^\alpha(x) - 2B_j(x) + e^{-\alpha h} B_{j+1}^\alpha(x)\right).$$

- defining $(\Delta_2^{h,\alpha}\boldsymbol{a})_j = e^{\alpha h} a_{j+1} - 2a_j + e^{-\alpha h} a_{j-1}$ we see that
- we can switch the difference $\displaystyle\sum_{j=1}^{m+2} a_j \Delta_2^{h,\alpha} B_j^\alpha(x) = \sum_{j=1}^{m+2} (\Delta_2^{h,\alpha}\boldsymbol{a})_j B_j^\alpha(x).$

Hyperbolic-polynomial Penalized Splines (HP-splines) [3]

Definition (Hyperbolic-polynomial Penalized Spline)

Given the data $(x_i, y_i)_{i=1,\dots,n}$ and the uniform knots $\Xi := \{a = \xi_1 < \xi_2 \cdots < \xi_m = b\}$, with $a \le x_1$, $x_n \le b$. Defined the exponential-polynomial B-splines $\{B_j^\alpha\}_{j=1}^{m+2}$ basis with segments in the space $E_{4,\alpha} := \mathrm{span}\{e^{\alpha x},\ x\, e^{\alpha x},\ e^{-\alpha x},\ x\, e^{-\alpha x}\}$, $\alpha \in \mathbb{R}$, the HPspline $s(x) = \sum_{j=1}^{m+2} a_j B_j^\alpha(x)$ is the solution of

$$\min_{a_1,\dots,a_{m+2}} \sum_{i=1}^{m} w_i \left(y_i - \sum_{j=1}^{m+2} a_j B_j^\alpha(x_i) \right)^2 + \lambda \sum_{j=1}^{m+2} \left((\Delta_2^{h,\alpha} \boldsymbol{a})_j \right)^2.$$

☞ HP-splines extend P-splines and reduce to them when $\alpha = 0$.

[3] R. Campagna, C. Conti, Penalized Hyperbolic-Polynomial Splines, Applied Mathematics Letters 118 (2021)

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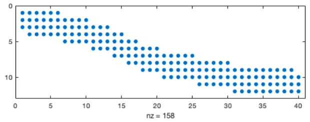
Hyperbolic-polynomial Penalized Splines (HP-splines)

The minimization problem is equivalent to solve the linear system

$$\mathrm{B}^T\mathrm{W}\mathrm{y} = \left(\mathrm{B}^T\mathrm{W}\mathrm{B} + \lambda(\mathrm{D}_2^{h,\alpha})^T\mathrm{D}_2^{h,\alpha}\right)\hat{a}, \quad \mathrm{B} := (B_j^\alpha(x_i))_{i=1,\dots,n}^{j=1,\dots,m+2}$$

where $\mathrm{y} \in \mathbb{R}^n$, $\mathrm{a} \in \mathbb{R}^{(m+2)}$, $\mathrm{B} \in \mathbb{R}^{m\times(m+2)}$, $\mathrm{W} \in \mathbb{R}^{n\times n}$, $\mathrm{D}_2^{h,\alpha} \in \mathbb{R}^{n\times(m+2)}$.

- B^T band structure is inherited by the B-splines locality and depends on the B-splines at the data x_j;
- $\mathrm{D}_2^{h,\alpha}$ is three-banded, with exponential terms depending on α.

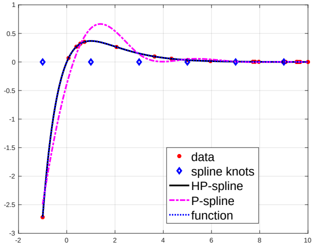


HP-spline properties (1)

1. P-splines P-splines **can fit constant and linear polynomial data exactly**:
   - cubic B-splines fit polynomial data up to degree 1
   - the reproduction property of the B-splines transfer to the P-splines, whatever the value of λ.

HP-splines $\mathbb{E}_{2,\alpha}$-reproduction

- hyperbolic-polynomial B-splines reproduce $\mathbb{E}_{2,\alpha}$
- the reproduction property of the *hyperbolic-polynomial* basis transfer to the HP-splines, whatever the value of λ.



HPspline properties (2)

1. P-splines **conserve** *pol.* **moments (mean, variance)** of the data:

$$\sum_{i=1}^{n} \hat{y}_i = \sum_{i=1}^{n} y_i \quad \textit{and} \quad \sum_{i=1}^{n} x_i \hat{y}_i = \sum_{i=1}^{n} x_i y_i,$$

with $\hat{y}_i = s(x_i) = \sum_{j=1}^{n+2} \hat{a}_j B_j(x_i)$ computed (predicted) values.

HP-splines conserve *exponential* **moments of the data**:

$$\sum_{i=1}^{n} e^{-\alpha x_i} \hat{y}_i = \sum_{i=1}^{n} e^{-\alpha x_i} y_i \quad \text{and} \quad \sum_{i=1}^{n} x_i e^{-\alpha x_i} \hat{y}_i = \sum_{i=1}^{n} x_i e^{-\alpha x_i} y_i.$$

HP-splines in action

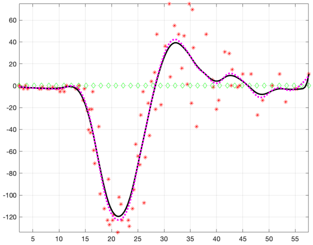
Numerical results

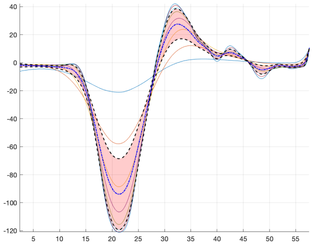
- **Test 1**: example of regression of a real dataset and comparison with P-spline.

- **Test 2**: Examples of working for different parameters:
  - sensitivity with respect to λ, α and the level of noise σ

Test 1: Benchmark Motorcycle Data

- L: HP-spline (black) vs P-spline (magenta), ($n = 40$, $\alpha = 0.3$ and $\lambda = 0.5$)
- R: HP-splines with $\alpha = 0.3$, $\lambda = 0.5$ and $n \in \{15, 20, 25, 30, 35, 40, 45, 50\}$. $n = 15$ and $n = 20$ grant a solution outside the 95% Bayesian conf. region.

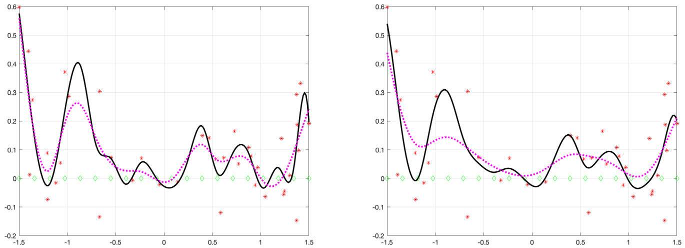


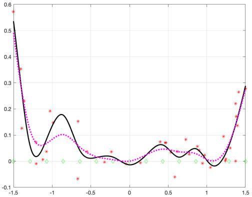


☞As expected, with no prior information, HP-spline behaves similarly to P-spline.

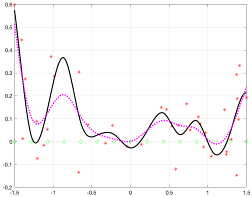
Test 2: comparison with Pspline on a *synthetic and noisy* data set

- Random $(x_i, y_i)_{i=1}^m$, with $m = 40$, $x_i \in [-1.5, 1.5]$, $y_i = f(x_i)$, $f(x) = 10^{-5}(e^{7x} - xe^{-7x})$, Gaussian noise with zero mean and st. dev. σ.
- Consider the HP-spline (black), with $\alpha = 3$.
- results for $n = 20$, $\sigma = 0.1$, $\lambda = 0.1$ (left) and $\lambda = 1$ (right).





$n = 15, \lambda = 0.1, \sigma = 5 \cdot 10^{-2}$



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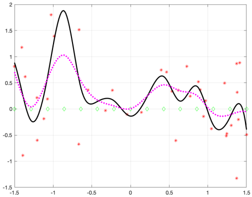

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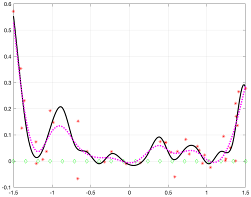

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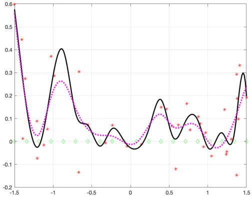

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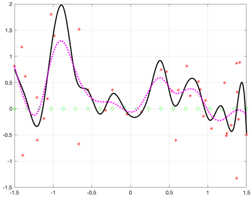

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Conclusions and Future work

- Splines are a simple but powerful tool that find application everywhere;
- According to the type of application polynomial splines must be replaced with other type of splines, for example exponential-polynomial splines;
- HP-splines inherit from P-splines the separation of the data from the free nodes avoiding the problems of overfitting, and boundary effects;
- HP-splines enjoy analogous properties of P-splines: moments preservation, exponential-polynomial reproduction;
- A clever selection of the frequency parameter α combined with a smart selection of λ is presently under investigation.

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Thank you for your attention!!