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Interpolation and linear prediction of data - three kernel selection criteria

Azzouz Dermoune¹, Mohammed Es.Sebaiy² and Jabrane Moustaaïd³
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Abstract

Interpolation and prediction have been useful approaches in modeling data in many areas of applications. The aim of this paper is the prediction of the next value of a time series (time series forecasting) using the techniques in interpolation of the spatial data, for the two approaches kernel interpolation and kriging. We are interested in finding some sufficient conditions for the kernels and provide a detailed analyse of the prediction using kernel interpolation. Finally, we provide a natural idea to select a good kernel among a given family of kernels using only the data. We illustrate our results by application to the data set on the mean annual temperature of France and Morocco recorded for a period of 115 years (1901 to 2015).

Keyword: Kernel interpolation, stochastic interpolation, linear algebra interpolation, cubic spline interpolation, climate change detection.

1 Introduction

Interpolation and prediction have been useful approaches in modelling data in many areas of applications such as the prediction of the meteorological variables, surface reconstruction and Interpolation of spatial data [1] among many more. For more details see [5], [6], [7] and [8]. In this work we extend the results of *Scheuerer* [1] to the linear prediction approach of time series. We also cite the work of *Dermoune et al* [2] where the parametrizations and the cubic spline were used as a model of prediction and we extend this results to the kernel interpolation framework.

Interpolation of spatial data is a very general mathematical problem and it's precise mathematical formulation as defined in [1] is to reconstruct a function $f : T \rightarrow \mathbb{R}$ with T is a domain in \mathbb{R}^d , based on its values at a finite set of data points $X = \{x_1, \dots, x_n\} \subset T$, the values $f(x_1), \dots, f(x_n)$ assumed to be known. But, in our case we are interested in the time series forecasting problem we have $T = \{x_1, \dots, x_n, x_{n+1}\}$ represent the time and the time series is $f(x_1), \dots, f(x_n)$ with the unknown value is $f(x_{n+1})$. In other words, we want to predict effectively the value $f(x_{n+1})$ using the known values $f(x_1), \dots, f(x_n)$. From [1]

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we have that both approaches kernel interpolation and kriging have the same approximant for the interpolation of spatial data problem, even with the different model assumption, a general overview in both approaches can be found in [9].

2 Linear prediction and kernel interpolation

Let $\mathbb{R}^{\{x_1, \dots, x_{n+1}\}}$ be the Hilbert space of real functions on $\{x_1, \dots, x_{n+1}\}$ with inner product (\cdot, \cdot) and norm $N(\cdot)$. The dual of $\mathbb{R}^{\{x_1, \dots, x_{n+1}\}}$ is spanned by the point evaluation linear forms $\delta_x : f \rightarrow f(x)$, $x \in \{x_1, \dots, x_{n+1}\}$, that is

$$(\mathbb{R}^{\{x_1, \dots, x_{n+1}\}})^* = (\delta_{x_1}, \dots, \delta_{x_{n+1}}).$$

Moreover, the dual norm N^* is defined by

$$(N^*(\mu))^2 = \sup\{|\mu(f)|^2 : N(f) \leq 1\},$$

for all $\mu \in (\mathbb{R}^{\{x_1, \dots, x_{n+1}\}})^*$.

Now, for any function $f \in \mathbb{R}^{\{x_1, \dots, x_{n+1}\}}$ and any sequence of real numbers (w_1, \dots, w_n) , we define the **linear prediction** of $f(x_{n+1})$

$$\hat{f}(x_{n+1}) = \sum_{i=1}^n w_i f(x_i),$$

with the error

$$\mathcal{Err}_n(f) := |f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i)|,$$

and the worst error in the unit ball w.r.t. the norm $N(\cdot)$

$$\mathcal{Werr}(f) := \sup\{|f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i)|^2 : N(f) \leq 1\} = (N^*(\delta_{x_{n+1}} - \sum_{i=1}^n w_i \delta_{x_i}))^2. \quad (1)$$

In the rest of this paper, we endow the vector space $\mathbb{R}^{\{x_1, \dots, x_{n+1}\}}$ with the scalar inner product

$$\begin{aligned} (f, f) &= (f, f)_{\mathbf{K}^{-1}} = \sum_{i=1}^{n+1} \sum_{j=1}^{n+1} f(x_i) f(x_j) k^{(-1)}(x_i, x_j) \\ &= \mathbf{f}^\top \mathbf{K}^{-1} \mathbf{f}, \end{aligned}$$

with $\mathbf{f} = (f(x_1), \dots, f(x_{n+1}))^\top$ and $\mathbf{K} = [k(x_i, x_j) : i, j = 1, \dots, n+1]$ is a fixed $(n+1) \times (n+1)$ symmetric positive definite matrix, with $k^{(-1)}(x_i, x_j)$ denotes the (i, j) entry of \mathbf{K}^{-1} . The norm defined by \mathbf{K} is given by $N(f) = \|\mathbf{K}^{-1/2} \mathbf{f}\|$, with $\|\cdot\|$ denotes the Euclidean norm.

2.1 Min-max prediction and kernel interpolation

Definition 2.1 (Min-max prediction). *A linear prediction $f^*(x_{n+1})$ of $f(x_{n+1})$ is called min-max if*

$$f^*(x_{n+1}) = \sum_{i=1}^n w_i^* f(x_i), \quad (2)$$

where (w_1^*, \dots, w_n^*) are given by the minimization of the $\mathcal{Werr}(f)$ 1.

The following result give us the optimal weights associate to the min-max prediction w.r.t. to the norm $\|\mathbf{K}^{-1/2} \cdot\|$.

Proposition 2.2. *The the worst error in the unit ball, $\mathcal{Werr}(f)$, w.r.t. to the norm $\|\mathbf{K}^{-1/2} \cdot\|$ is equals*

$$\mathcal{Werr}(f) = \|\delta_{x_{n+1}} - \sum_{i=1}^n w_i \delta_{x_i}\|_{\mathbf{K}^{1/2}}^2 \quad (3)$$

where $\|\cdot\|_{\mathbf{K}^{1/2}}$ denotes the dual norm defined by the dual scalar inner product

$$(\delta_{x_i}, \delta_{x_j})_{\mathbf{K}} = k(x_i, x_j), \quad i, j = 1, \dots, n+1.$$

Proof. From the general theory of reproducing kernel Hilbert spaces, see [9, 1], we have

$$\begin{aligned} & \sup_{\|\mathbf{K}^{-1/2} \mathbf{f}\| \leq 1} \left\{ \left| f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i) \right|^2 \right\} \\ &= \sup_{\|\mathbf{K}^{-1/2} \mathbf{f}\| \leq 1} \left\{ [\mathbf{K}^{-1/2} \mathbf{f}]^\top [\mathbf{K}^{1/2}(-w_1, \dots, -w_n, 1)^\top (-w_1, \dots, -w_n, 1) \mathbf{K}^{1/2}] [\mathbf{K}^{-1/2} \mathbf{f}] \right\} \\ &= \text{the largest eigenvalue of } [\mathbf{K}^{1/2}(-w_1, \dots, -w_n, 1)^\top (-w_1, \dots, -w_n, 1) \mathbf{K}^{1/2}] \\ &= \|\mathbf{K}^{1/2}(-w_1, \dots, -w_n, 1)^\top\|^2 = (-w_1, \dots, -w_n, 1) \mathbf{K} (-w_1, \dots, -w_n, 1)^\top \\ &= \|\delta_{x_{n+1}} - \sum_{i=1}^n w_i \delta_{x_i}\|_{\mathbf{K}^{1/2}}^2. \end{aligned}$$

□

Corollary 2.3. *The optimal weights of the min-max linear prediction of $f(x_{n+1})$ are given by*

$$\mathbf{w}^* = (w_1^*, \dots, w_n^*) = [k(x_{n+1}, x_1), \dots, k(x_{n+1}, x_n)] [k(x_i, x_j) : i, j = 1, \dots, n]^{-1}. \quad (4)$$

Proof. The optimal weights are given by the minimization

$$\arg \min \left\{ \left\| \delta_{x_{n+1}} - \sum_{i=1}^n w_i \delta_{x_i} \right\|_{\mathbf{K}^{1/2}}^2 : w_1, \dots, w_n \in \mathbb{R} \right\}, \quad (5)$$

which is the solution of the system

$$\sum_{j=1}^n w_j k(x_i, x_j) = k(x_{n+1}, x_i), \quad i = 1, \dots, n, \quad (6)$$

it follows easily that \mathbf{w}^* is given by 4. \square

Remarks 2.4. 1) *The worst case linear prediction error in the ball with the radius $r > 0$ w.r.t. to the norm $\|\mathbf{K}^{-1/2} \cdot\|$ is equal to*

$$\begin{aligned} & \sup_{\|\mathbf{K}^{-1/2} \mathbf{f}\| \leq r} \{ |f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i)|^2 \} \\ & = r^2 (-w_1, \dots, -w_n, 1) \mathbf{K} (-w_1, \dots, -w_n, 1)^\top, \end{aligned}$$

as a result the optimal weights (4) do not depend on the radius of the ball.

2) *The prediction using the spline interpolating w.r.t. the norm $\|\mathbf{K}^{-1/2} \cdot\|$ (see, e.g., [9]) defined by the minimizer :*

$$S(f) = \arg \min \{ \|\mathbf{K}^{-1/2} \mathbf{f}\| : f(x_1), \dots, f(x_n) \text{ are fixed} \},$$

coincide with the prediction (2).

3) *The min-max prediction (2) is equal to*

$$f^*(x_{n+1}) = \sum_{j=1}^n \alpha_j^* k(x_{n+1}, x_j), \quad (7)$$

where $\alpha_j^, j = 1, \dots, n$ is the solution of the system*

$$\sum_{j=1}^n \alpha_j^* \mathbf{k}(x_i, x_j) = f(x_i), \quad i = 1, \dots, n, \quad (8)$$

Now, we turn to the interpolation of the function f at the set $\{x_1, \dots, x_n\}$ using $\text{span}(\mathbf{k}_1, \dots, \mathbf{k}_n)$ where \mathbf{k}_j denotes the j -th column of the matrices \mathbf{K} . Then the interpolation of the function f equals

$$I(f) = \sum_{j=1}^n \alpha_j^* \mathbf{k}_j$$

with the weights α^* are given by (8). The following Proposition gives the error of interpolation.

Proposition 2.5 (Interpolation error). *The error of interpolation, \mathcal{IErr} , is given by*

$$\mathcal{IErr}(f) := f(x_{n+1}) - f^*(x_{n+1}) = [\mathbf{k}_{n+1}^{(-1)} \mathbf{f}] [k(x_{n+1}, x_{n+1}) - \sum_{i=1}^n w_i^* k(x_i, x_{n+1})]. \quad (9)$$

Proof. First, observe that we can write the coordinates of \mathbf{f} in the basis \mathbf{K} as

$$\mathbf{f} = \sum_{j=1}^{n+1} [\mathbf{k}_j^{(-1)} \mathbf{f}] \mathbf{k}_j.$$

with $\mathbf{k}_j^{(-1)}$ denotes the j -th row of \mathbf{K}^{-1} . Therefore

$$\begin{aligned} I(f) &= \sum_{j=1}^{n+1} [\mathbf{k}_j^{(-1)} \mathbf{f}] I(\mathbf{k}_j) \\ &= \sum_{j=1}^n [\mathbf{k}_j^{(-1)} \mathbf{f}] \mathbf{k}_j + [\mathbf{k}_{n+1}^{(-1)} \mathbf{f}] I(\mathbf{k}_{n+1}), \end{aligned}$$

because the interpolation of \mathbf{k}_j is exact for $j = 1, \dots, n$. Thus,

$$\begin{aligned} f - I(f) &= [\mathbf{K}_{n+1}^{-1} \mathbf{f}] (\mathbf{k}_{n+1} - I(\mathbf{k}_{n+1})) \\ &= [\mathbf{k}_{n+1}^{(-1)} \mathbf{f}] (0, \dots, 0, [k(x_{n+1}, x_{n+1}) - \sum_{i=1}^n w_i^* k(x_i, x_{n+1})])^\top, \end{aligned}$$

which completes the proof. \square

2.2 Min-max linear prediction with constraint

In this section, we consider the optimization (5) under the constraint

$$\sum_{i=1}^n w_i \mathbf{p}_k(x_i) = \mathbf{p}_k(x_{n+1}), \quad k = 1, \dots, q, \quad (10)$$

where $\mathbf{p}_1, \dots, \mathbf{p}_q \in \mathbb{R}^{\{x_1, \dots, x_{n+1}\}}$ are given.

Solve the minimization (5) under the constraint (10) is equivalent to solve the system

$$\begin{cases} \sum_{j=1}^n k(x_i, x_j) w_j + \sum_{k=1}^q \lambda_k \mathbf{p}_k(x_i) = k(x_i, x_{n+1}), & i = 1, \dots, n, \\ \sum_{j=1}^n w_j \mathbf{p}_k(x_j) = \mathbf{p}_k(x_{n+1}), & k = 1, \dots, q, \end{cases} \quad (11)$$

where $\lambda_1, \dots, \lambda_q$ are the Lagrange multiplier. The solution is unique if the homogeneous system

$$\begin{aligned} \sum_{j=1}^n k(x_i, x_j) w_j + \sum_{k=1}^q \lambda_k \mathbf{p}_k(x_i) &= 0, \quad i = 1, \dots, n, \\ \sum_{j=1}^n w_j \mathbf{p}_k(x_j) &= 0, \quad k = 1, \dots, q, \end{aligned}$$

has a unique solution $w_1 = \dots = w_n = 0$, $\lambda_1 = \dots = \lambda_q = 0$. This is equivalent to say that the columns $(p_k(x_1), \dots, p_k(x_n))^\top$, $k = 1, \dots, q$, are linearly independent and that \mathbf{K} is conditionally positive w.r.t. $\mathbf{p}_1, \dots, \mathbf{p}_q$, i.e. the system

$$\sum_{j=1}^n \sum_{i=1}^n k(x_i, x_j) w_j w_i = 0, \quad \sum_{i=1}^n w_i p_k(x_i) = 0, \quad k = 1, \dots, q,$$

has a unique solution $w_1 = \dots = w_n = 0$. Observe that this is true if \mathbf{K} is definite positive, but it is not necessary.

Let w_1^*, \dots, w_n^* , $\lambda_1^*, \dots, \lambda_q^*$ be the solution of the system (11). Then the optimal prediction under the constraint (10) is

$$f^*(x_{n+1}) = \sum_{i=1}^n w_i^* f(x_i). \quad (12)$$

Constraint's parametrization

Now, let $\mathbf{z}^{(1)} = (z_1^{(1)}, \dots, z_n^{(1)})^\top$ be a particular solution of the system (10) and $\mathbf{z}_1 = (z_{11}, \dots, z_{n1})^\top$, \dots , $\mathbf{z}_{n-q} = (z_{1n-q}, \dots, z_{nn-q})^\top$, $n - q$ independent solutions of the corresponding homogeneous system. Then the general solution of the system (10) has the form

$$\mathbf{w} = \mathbf{z}^{(1)} + \sum_{l=1}^{n-q} \tilde{w}_l \mathbf{z}_l.$$

Let us consider the basis

$$\begin{aligned} \mathbf{B} &= [\mathbf{p}_1, \dots, \mathbf{p}_q, \sum_{i=1}^n z_{i1} \mathbf{k}_i, \dots, \sum_{i=1}^n z_{in-q} \mathbf{k}_i, \mathbf{b}_{n+1}] \\ &=: [\mathbf{b}_1, \dots, \mathbf{b}_{n+1}] \end{aligned} \quad (13)$$

such that the expansion of \mathbf{f} in the basis \mathbf{B} is given by

$$\mathbf{f} = \sum_{l=1}^q \theta_l \mathbf{f} \mathbf{p}_l + \sum_{l=1}^{n-q} \theta_{q+l} \mathbf{f} \mathbf{b}_{q+l} + \theta_{n+1} \mathbf{f} \mathbf{b}_{n+1},$$

with $\theta_{n+1} = (-(\mathbf{z}^{(1)})^\top, 1)$.

The unknowns are the rows $\theta_1, \dots, \theta_n$, and the column \mathbf{b}_{n+1} . They are solution of the system

$$\begin{aligned} \delta(i = j) &= \sum_{l=1}^q p_l(x_i) \theta_{lj} + \sum_{l=1}^{n-q} b_{q+l}(x_i) \theta_{(q+l)j} + b_{n+1}(x_i) \theta_{(n+1)j} \\ i, j &= 1, \dots, n+1. \end{aligned} \quad (14)$$

The interpolation of any function g at the set $\{x_1, \dots, x_n\}$ using $\text{span}(\mathbf{b}_1, \dots, \mathbf{b}_n)$ is given by the map

$$I(g) = \sum_{j=1}^n \beta_j \mathbf{b}_j,$$

with β is the solution of the system

$$\sum_{j=1}^n \beta_j \mathbf{b}_j(x_i) = g(x_i), \quad i = 1, \dots, n.$$

Using similar arguments as in proposition 2.5, we can deduce the following result.

Proposition 2.6. *The value*

$$\sum_{j=1}^n z_j^{(1)} k(x_j, x_{n+1}) + I(f - \sum_{j=1}^n z_j^{(1)} \mathbf{k}_j)(x_{n+1})$$

coincides with $f^(x_{n+1})$ given by (12). In addition, the error is equal to*

$$\begin{aligned} f(x_{n+1}) - f^*(x_{n+1}) &= f(x_{n+1}) - \sum_{j=1}^n z_j^{(1)} k(x_j, x_{n+1}) - I(f - \sum_{j=1}^n z_j^{(1)} \mathbf{k}_j)(x_{n+1}) \\ &= [\mathbf{b}_{n+1}^{(-1)}(f - \sum_{j=1}^n z_j^{(1)} \mathbf{k}_j)][b_{n+1}(x_{n+1}) - I(\mathbf{b}_{n+1})(x_{n+1})]. \end{aligned}$$

If \mathbf{K} is invertible and $\mathbf{p}_l = \mathbf{k}_l$ with $l = 1, \dots, n$, then $\theta_l = \mathbf{k}_l^{(-1)}$ for $l = 1, \dots, n$, and the basis (14) is given by $\mathbf{b}_l = \mathbf{k}_l$ with $l = 1, \dots, n$, and $\mathbf{b}_{n+1} = \frac{\mathbf{k}_{n+1}}{k(x_{n+1}, x_{n+1}) - I(\mathbf{k}_{n+1})(x_{n+1})}$.

Constraint's effect on the kernel

From the notations above the general solution of the system (10) has the form

$$\mathbf{w} = \mathbf{z}^{(1)} + \sum_{l=1}^{n-q} \tilde{w}_l \mathbf{z}_l.$$

As a consequence the quadratic form

$$\|\delta_{x_{n+1}} - \sum_{i=1}^n w_i \delta_{x_i}\|_{\mathbf{K}}^2 = \|\mu_{n+1-q} - \sum_{l=1}^{n-q} \tilde{w}_l \mu_l\|_{\tilde{\mathbf{K}}}^2,$$

with $\mu_1 = \sum_{i=1}^n z_{i1} \delta_{x_i}$, \dots , $\mu_{n-q} = \sum_{i=1}^n z_{i, n-q} \delta_{x_i}$, $\mu_{n+1-q} = \delta_{x_{n+1}} - \sum_{i=1}^n z_i^{(1)} \delta_{x_i}$, and the entries of the $(n+1-q) \times (n+1-q)$ kernel $\tilde{\mathbf{K}}$ are given by

$$\tilde{k}(l_1, l_2) = (\mu_{l_1}, \mu_{l_2})_{\mathbf{K}}, \quad l_1, l_2 = 1, \dots, n+1-q.$$

Observe that $\tilde{\mathbf{K}}$ is positive definite if and only if the columns $(p_k(x_1), \dots, p_k(x_n))^\top$, $k = 1, \dots, q$, are linearly independent and \mathbf{K} is conditionally positive w.r.t. $\mathbf{p}_1, \dots, \mathbf{p}_q$. It follows that

$$\begin{aligned} & \sup\{|f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i)|^2 : \tilde{f}^\top \tilde{\mathbf{K}}^{-1} \tilde{f} \leq 1\} \\ &= \|\mu_{n+1-q} - \sum_{l=1}^{n-q} \tilde{w}_l \mu_l\|_{\tilde{\mathbf{K}}}^2, \end{aligned}$$

where $\tilde{f} = (\tilde{f}(1), \dots, \tilde{f}(n+1-q))^\top \in \mathbb{R}^{n+1-q}$ are defined by

$$\begin{aligned} \tilde{f}(1) &= \sum_{i=1}^n z_{i1} f(x_i), \dots, \tilde{f}(n-q) = \sum_{i=1}^n z_{in-q} f(x_i), \\ \tilde{f}(n+1-q) &= f(x_{n+1}) - \sum_{i=1}^n z_i^{(1)} f(x_i). \end{aligned}$$

The map $f \in \mathbb{R}^{\{x_1, \dots, x_{n+1}\}} \rightarrow \tilde{f}^\top \tilde{\mathbf{K}}^{-1} \tilde{f}$ is a semi kernel having the null space spanned by $\mathbf{p}_1, \dots, \mathbf{p}_q$.

That being the case, the optimal weights \tilde{w}^* are given by

$$\tilde{w}^* = \arg \min\{\|\mu_{n+1-q} - \sum_{l=1}^{n-q} \tilde{w}_l \mu_l\|_{\tilde{\mathbf{K}}}^2 : \tilde{w}_1, \dots, \tilde{w}_{n-q} \in \mathbb{R}\},$$

and then predict $f(x_{n+1})$ is equal to

$$\sum_{i=1}^n z_i^{(1)} f(x_i) + \sum_{l=1}^{n-q} \tilde{w}_l^* \left(\sum_{i=1}^n z_{il} f(x_i) \right).$$

The latter predictor coincides with (12). Moreover, the spline

$$S(\tilde{f}) = \arg \min_{\tilde{f}(n+1-q)} \{ \tilde{f}^\top \tilde{\mathbf{K}}^{-1} \tilde{f} : \tilde{f}(1), \dots, \tilde{f}(n-q) \text{ are fixed} \}$$

is such that

$$S(\tilde{f})(n+1-q) = f^*(x_{n+1}) - \sum_{i=1}^n z_i^{(1)} f(x_i)$$

with $f^*(x_{n+1})$ is the optimal prediction under the constraint (12).

From the expansion of \mathbf{f} in the basis $\mathbf{B} = [\mathbf{b}_1, \dots, \mathbf{b}_{n+1}]$ (13), we can conclude the following result.

Proposition 2.7. *If the weights w satisfy the constraint (10), then*

$$|f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i)|^2 = \left| \sum_{l=1}^{n+1-q} \tilde{f}_l \{b_{q+l}(x_{n+1}) - \sum_{i=1}^n w_i b_{q+l}(x_i)\} \right|^2.$$

It follows that

$$\begin{aligned} & \sup \left\{ \left| f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i) \right|^2 : \tilde{f}^\top \tilde{\mathbf{K}}^{-1} \tilde{f} \leq 1 \right\} \\ &= (b_{q+1}(x_{n+1}) - \sum_{i=1}^n w_i b_{q+1}(x_i), \dots, b_{n+1}(x_{n+1}) - \sum_{i=1}^n w_i b_{n+1-q}(x_i)) \tilde{\mathbf{K}}^{-1} \\ & (b_{1+q}(x_{n+1}) - \sum_{i=1}^n w_i b_{1+q}(x_i), \dots, b_{n+1}(x_{n+1}) - \sum_{i=1}^n w_i b_{n+1}(x_i))^\top \\ &= (-w_1, \dots, -w_n, 1) \mathbf{R} \tilde{\mathbf{K}} \mathbf{R}^\top (-w_1, \dots, -w_n, 1)^\top \\ &= (-\tilde{w}_1, \dots, -\tilde{w}_{n-q}, 1) \tilde{K} (-\tilde{w}_1, \dots, -\tilde{w}_{n-q}, 1)^\top \\ &= \left\| \mu_{n+1-q} - \sum_{l=1}^{n-q} \tilde{w}_l \mu_l \right\|_{\tilde{\mathbf{K}}}^2, \end{aligned}$$

with the $(n+1) \times (n+1-q)$ matrix

$$\mathbf{R} = [\mathbf{b}_{q+1}, \dots, \mathbf{b}_{n+1}].$$

2.3 Semi-kernel and constraint

Now, conversely we consider a semi-kernel Q on $\mathbb{R}^{\{x_1, \dots, x_{n+1}\}}$ with the null space spanned by q functions p_1, \dots, p_q and let

$$S(f) = \arg \min \{Q(f, f) : f(x_1), \dots, f(x_n) \text{ are fixed}\}$$

be the spline defined by the semi-norm Q , and

$$S(f)(x_{n+1}) = \sum_{i=1}^n w_i^* f(x_i).$$

We consider a basis $\mathbf{B} = [\mathbf{b}_1, \dots, \mathbf{b}_{n+1}]$ such that $\mathbf{b}_l = \mathbf{p}_l$ with $l = 1, \dots, q$ and let $(\theta_1, \dots, \theta_q, u_1, \dots, u_{n+1-q})$ be the coordinates of \mathbf{f} , i.e.

$$\mathbf{f} = \sum_{l=1}^q \theta_l \mathbf{p}_l + \sum_{l=1}^{n+1-q} u_l \mathbf{b}_{q+l}.$$

It follows that

$$Q(f, f) = \sum_{l_1=1}^{n+1-q} \sum_{l_2=1}^{n+1-q} u_{l_1} u_{l_2} Q(\mathbf{b}_{q+l_1}, \mathbf{b}_{q+l_2}) = \|Q^{1/2} \mathbf{u}\|^2,$$

and the kernel $Q = [Q_{l_1, l_2} : l_1, l_2 = 1, \dots, n+1-q]$ is invertible. If the weights \mathbf{w} satisfy the constraint (10), then

$$|f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i)|^2 = \left| \sum_{l=1}^{n+1-q} u_l \{b_l(x_{n+1}) - \sum_{i=1}^n w_i b_l(x_i)\} \right|^2,$$

therefore,

$$\begin{aligned} & \sup \left\{ \left| f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i) \right|^2 : Q(\mathbf{f}, \mathbf{f}) \leq 1 \right\} \\ &= \sup \left\{ \left| f(x_{n+1}) - \sum_{i=1}^n w_i f(x_i) \right|^2 : \mathbf{u}^\top Q \mathbf{u} \leq 1 \right\} \\ &= (b_{q+1}(x_{n+1}) - \sum_{i=1}^n w_i b_{q+1}(x_i), \dots, b_{n+1}(x_{n+1}) - \sum_{i=1}^n w_i b_{n+1-q}(x_i)) Q^{-1} \\ & \quad (b_{1+q}(x_{n+1}) - \sum_{i=1}^n w_i b_{1+q}(x_i), \dots, b_{n+1}(x_{n+1}) - \sum_{i=1}^n w_i b_{n+1}(x_i))^\top \\ &= (-w_1, \dots, -w_n, 1) \mathbf{R} Q^{-1} \mathbf{R}^\top (-w_1, \dots, -w_n, 1)^\top, \end{aligned}$$

where the $(n+1) \times (n+1-q)$ matrix

$$\mathbf{R} = [b_{q+1}, \dots, b_{n+1}].$$

3 Stochastic approach

The statistical counterpart to the kernel interpolation is known as kriging (see e.g. [1]). It is based on the modeling assumption that $(f(x_1), \dots, f(x_n), f(x_{n+1}))$ is a realization of random vector $Y_{x_1}, \dots, Y_{x_{n+1}}$ over the same probability space $(\Omega, \mathcal{F}, \mathbf{P})$. To predict $Y_{x_{n+1}}$ known Y_{x_1}, \dots, Y_{x_n} we need the mean and the covariance matrix of the random vector $(Y_{x_1}, \dots, Y_{x_{n+1}})$. We assume that the mean $(m(x_1), \dots, m(x_{n+1}))$ (also called the trend) and the covariance function

$$k(x_i, x_j) = \text{cov}(Y_{x_i}, Y_{x_j})$$

of the random vector $(Y_{x_1}, \dots, Y_{x_{n+1}})$ exist.

If Y_{x_1}, \dots, Y_{x_n} are assumed to be known, then the best linear unbiased predictor (BLUP) of $Y_{x_{n+1}}$ is given by

$$\hat{Y}_{x_{n+1}} = \sum_{i=1}^n w_i^* Y_{x_i},$$

where the weights w_i^* are the solution of the following optimization problem

$$\min \left\{ \text{var}(Y_{x_{n+1}} - \sum_{i=1}^n w_i Y_{x_i}) : w_1, \dots, w_n \in \mathbb{R}, \sum_{i=1}^n w_i m(x_i) = m(x_{n+1}) \right\}. \quad (15)$$

If the mean function m is modeled as

$$m(x_i) = \sum_{k=1}^q \beta_k p_k(x_i) : \quad i = 1, \dots, n+1,$$

and if we consider the weights such that

$$\sum_{i=1}^n w_i p_l(x_i) = p_l(x_{n+1}), \quad l = 1, \dots, q,$$

then the optimal predictor

$$\hat{f}(x_{n+1}) = \sum_{i=1}^n w_i^* f(x_i)$$

of $f(x_{n+1})$ in stochastic sense coincides with the interpolation (12).

4 Three kernel selection criteria

Kernel interpolation and prediction approaches are based on the knowledge of a symmetric positive definite matrix \mathbf{K} and the trend $\mathbf{p}_1, \dots, \mathbf{p}_q$. To apply kernel interpolation it amounts to the assumption that one knows the degree of smoothness of the function f . In the context of partial differential equations, the function f belongs to some Sobolev space. In stochastic approach the covariance matrix and the trend are chosen using the maximum likelihood method or the Bayesian method.

Here we propose three natural criteria to compare two kernels $\mathbf{K}^{(1)}$ and $\mathbf{K}^{(2)}$. Known $f(x_1), \dots, f(x_r)$, we predict $f(x_{r+1})$ using the kernel $[k^{(l)}(i, j) : i, j = 1, \dots, r]$, and we obtain the predictor $\hat{f}^{(l)}(x_{r+1})$, with $l = 1, 2$, and $r = 2, \dots, n-1$. We propose the following three criteria to measure the performance of the Kernel $\mathbf{K}^{(l)}$:

1) $MSPE(l) =: \frac{\sum_{j=1}^{n-1} |f(x_{j+1}) - \hat{f}^{(l)}(x_{j+1})|^2}{n-1}$. We say that $\mathbf{K}^{(1)}$ is better than $\mathbf{K}^{(2)}$ w.r.t. the MSPE criterion if

$$MSPE(1) < MSPE(2).$$

2) $MAXPE(l) =: \max\{|f(x_{j+1}) - \hat{f}^{(l)}(x_{j+1})| : j = 1, \dots, n-1\}$. We say that $\mathbf{K}^{(1)}$ is better than $\mathbf{K}^{(2)}$ w.r.t. the MAXPE criterion if

$$MAXPE(1) < MAXPE(2).$$

3) We say that $\mathbf{K}^{(1)}$ is statistically better than $\mathbf{K}^{(2)}$ if

$$\frac{\sum_{j=1}^{n-1} \mathbf{1}_{[|f(x_{j+1}) - \hat{f}^{(1)}(x_{j+1})| < |f(x_{j+1}) - \hat{f}^{(2)}(x_{j+1})|]}}{n-1} > 1/2.$$

These criteria were also used in [?].

5 Application

In the climate change problem we are interested in the mean temperature $f(t)$ at the time t . The data are the years taken into account $t_1 < \dots < t_{n+1}$ and the mean temperature $f(t_1), \dots, f(t_n)$, and we are interested in the prediction of $f(t_{n+1})$. We recall that

$$\arg \min \left\{ \int_{t_1}^{t_{n+1}} |g''(t)|^2 dt : g(t_1) = f(t_1), \dots, g(t_{n+1}) = f(t_{n+1}) \text{ are fixed} \right\}$$

is the natural C^2 cubic spline s which interpolates the points $(t_i, f(t_i)), i = 1, \dots, n+1$. See [10, 11]. We assume that $f(t_1), \dots, f(t_{n+1})$ are the values of a natural C^2 cubic spline. We are going to predict $f(t_{n+1})$ using three kernels, and we need some notations.

5.1 Kernel and semikernels using cubic splines

Let $S = S_3(t_1, \dots, t_{n+1})$ be the set of C^2 cubic splines having the knots $t_1 < \dots < t_{n+1}$. Note that every element $s \in S$ is a C^2 map on $[t_1, t_{n+1}]$ and is a polynomial of degree three on each interval $[t_i, t_{i+1})$ for $i = 1, \dots, n$.

More precisely, let

$$\begin{aligned} p_1 &= s(t_1), \dots, p_{n+1} = s(t_{n+1}), & q_1 &= s'(t_1), \dots, q_{n+1} = s'(t_{n+1}), \\ u_1 &= s''(t_1), \dots, u_{n+1} = s''(t_{n+1}), & v_1 &= s'''(t_1+), \dots, v_n = s'''(t_n+) \end{aligned}$$

be respectively the values of s and its derivatives up to order three at the knots. We have for every $i = 1, \dots, n$,

$$s(t) = p_i + q_i(t - t_i) + (t - t_i)^2 u_i / 2 + (t - t_i)^3 v_i / 6, \quad t \in [t_i, t_{i+1}).$$

The following constraint for $h_i = t_{i+1} - t_i, i = 1, \dots, n$ ensures the hypothesis that s is C^2 :

$$p_i + q_i h_i + u_i h_i^2 / 2 + v_i h_i^3 / 6 = p_{i+1}, \quad (16)$$

$$q_i + u_i h_i + v_i h_i^2 / 2 = q_{i+1}, \quad (17)$$

$$v_i = s^{(3)}(t_i) = (u_{i+1} - u_i) / h_i. \quad (18)$$

It is well known (see [?]) that S has the dimension $n+3$, and the set of natural spline S_{nat} has the dimension $n+1$. Hence an element $s \in S$ (respectively $s \in S_{nat}$) is completely defined by $n+3$ (respectively $n+1$ parameters) independent parameters.

Now we need to parametrize the set S in order to define properly an element $s \in S$. A parametrization of S is a one-to-one linear map

$$\Theta : s \in S \rightarrow \theta \in \mathbb{R}^{n+3}.$$

Defining a parametrization Θ is equivalent to the existence of the basis $\mathbf{B} = (\mathbf{b}_1, \dots, \mathbf{b}_{n+3})$ of S such that, for all $s \in S$,

$$s = \sum_{i=1}^{n+3} \theta_i \mathbf{b}_i = \mathbf{B}\theta.$$

The parametrization $\Theta_{002} = (p_1, p_2, u_1, \dots, u_{n+1})$ defines the basis $\mathbf{B}_{002} = (\mathbf{b}_1^{002}, \dots, \mathbf{b}_{n+3}^{002})$. The subscript notation 002 is justified by the fact that

$$\begin{aligned} p_1 &= s(t_1) = s^{(0)}(t_1), p_2 = s(t_2) = s^{(0)}(t_2), \\ u_1 &= s''(t_1) = s^{(2)}(t_1), \dots, u_{n+1} = s''(t_{n+1}) = s^{(2)}(t_{n+1}). \end{aligned}$$

See [2, 3, 4] for more details.

It follows for $s \in S_{nat}$ that

$$s = p_1 \mathbf{b}_1^{002} + p_2 \mathbf{b}_2^{002} + \sum_{i=2}^n u_i \mathbf{b}_{2+i}^{002},$$

and then $\mathbf{s} = (s(t_1), \dots, s(t_{n+1}))^\top$ is given by

$$\mathbf{s} = [\mathbf{b}_1^{002}(\mathbf{t}), \mathbf{b}_2^{002}(\mathbf{t})](p_1, p_2)^\top + \sum_{i=2}^n \mathbf{R}(u_2, \dots, u_n)^\top,$$

Here the column $\mathbf{b}_i^{002}(\mathbf{t}) = (b_i^{002}(t_1), \dots, b_i^{002}(t_{n+1}))^\top$, with $i = 4, \dots, n+2$, and the $n+1 \times n+1$ matrix

$$\mathbf{R} = [\mathbf{b}_4^{002}(\mathbf{t}), \dots, \mathbf{b}_{n+2}^{002}(\mathbf{t})].$$

Observe that $\text{span}(\mathbf{b}_1^{002}, \mathbf{b}_2^{002}) = \text{span}(\mathbf{1}, \mathbf{t})$ with the column $\mathbf{1} = (1, \dots, 1)^\top$, $\mathbf{t} = (t_1, \dots, t_{n+1})^\top$.

We can show that

$$\begin{aligned} & \int_{t_1}^{t_{n+1}} |s''(t)|^2 dt = \\ & \sum_{i=1}^n \int_{t_i}^{t_{i+1}} |u_i + t(u_{i+1} - u_i)/h_i|^2 dt \\ &= \sum_{i=1}^n (u_i^2 + u_i u_{i+1} + u_{i+1}^2) h_i / 3 \\ &= (u_2, \dots, u_n) \mathbf{Q} (u_2, \dots, u_n)^\top, \end{aligned} \tag{19}$$

with \mathbf{Q} is a known $n-1 \times n-1$ invertible matrix see [2]. We also recall that

$$(u_2, \dots, u_n)^\top = \mathbf{U}(p_1, \dots, p_{n+1})^\top,$$

with \mathbf{U} is a known $n - 1 \times n + 1$ matrix see [2]. Therefore

$$(u_2, \dots, u_n) \mathbf{Q} (u_2, \dots, u_n)^\top = (p_1, \dots, p_{n+1}) \mathbf{U}^\top \mathbf{Q} \mathbf{U} (p_1, \dots, p_{n+1})^\top \quad (20)$$

$$=: (p_1, \dots, p_{n+1}) \mathbf{P} (p_1, \dots, p_{n+1})^\top \quad (21)$$

$$(22)$$

Now we propose the following predictors for $f(t_{n+1})$.

0) We assume that \mathbf{s} is Gaussian centred with the covariance matrix $\mathbf{K}^{(0)} = (\mathbf{Q}^{(0)})^{-1}$ with $\mathbf{Q}^{(0)}$ is defined by

$$\int_{t_1}^{t_{n+1}} |s(t)|^2 dt = \mathbf{s}^\top \mathbf{Q}^{(0)} \mathbf{s}.$$

1) We consider the spline

$$S(f) = \arg \min \{ (f(t_1), \dots, f(t_{n+1})) \mathbf{P} (f(t_1), \dots, f(t_{n+1}))^\top : f(t_1), \dots, f(t_n) \text{ are fixed} \}, (23)$$

defined by the kernel \mathbf{P} (21) and the predictor $f^*(t_{n+1}) = S(f)(t_{n+1})$ of $f(t_{n+1})$. We assume that \mathbf{s} is Gaussian with the mean $p_1 \mathbf{b}_1^{002}(\mathbf{t}) + p_2 \mathbf{b}_2^{002}(\mathbf{t}) = \beta_1 \mathbf{1} + \beta_1 \mathbf{t}$ and the covariance matrix $\mathbf{K}^{(1)} = \mathbf{R} \mathbf{Q}^{-1} \mathbf{R}^\top$ with the kernel \mathbf{Q} is given by (20). The predictor $\hat{f}^{(1)}(t_{n+1})$ of $f(t_{n+1})$ (12) using the kernel $\mathbf{K}^{(1)}$ coincides with $S(f)(t_{n+1})$.

2) We assume that \mathbf{s} is Gaussian with the mean $p_1 \mathbf{b}_1^{002}(\mathbf{t}) + p_2 \mathbf{b}_2^{002}(\mathbf{t}) = \beta_1 \mathbf{1} + \beta_1 \mathbf{t}$ and the covariance matrix $\mathbf{K}^{(2)} = \mathbf{R} \mathbf{Q} \mathbf{R}^\top$.

Let $\hat{f}^{(i)}(t_{n+1})$ be the predictor of $f(t_{n+1})$ (12) using the kernel $\mathbf{K}^{(i)}$ with $i = 0, 1, 2$. Using real data, we are going to compare these three predictors.

5.2 Real data Application

As application in the climate change area we are interested in the annual mean temperature observed in France and Morocco from 1901 to 2015, the data are presented in Figure 1. We illustrate the importance of the kernel choice by considering the kernels $\mathbf{K}^{(0)}$, $\mathbf{K}^{(1)}$, $\mathbf{K}^{(2)}$. The three kernel selection criteria are presented in Table 1. The mean annual temperature of the year 2015 and 2016 (i.e. $\hat{f}^{(i)}(t_n)$ and $\hat{f}^{(i)}(t_{n+1})$, $n = 114$) are given in Tables (2, 3), as for Figure 2 it shows the splines of the predictors $\hat{f}^{(0)}$, $\hat{f}^{(1)}$, $\hat{f}^{(2)}$ and the true temperature. The w_1^*, \dots, w_n^* of (12) for the kernels $\mathbf{K}^{(0)}$, $\mathbf{K}^{(1)}$, $\mathbf{K}^{(2)}$ are presented in Figure 3.

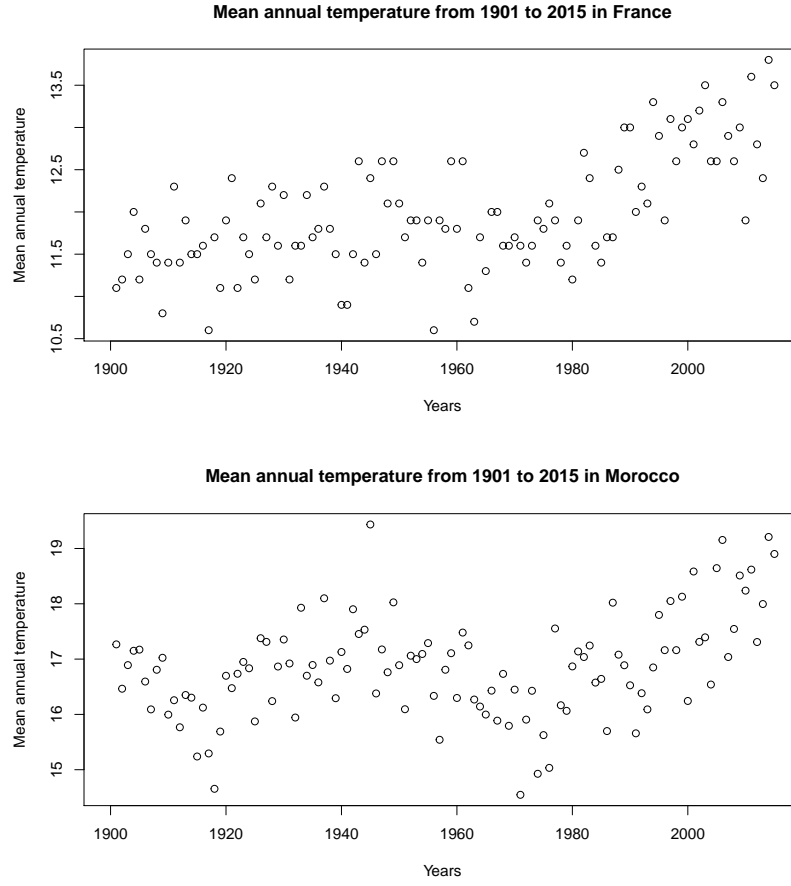


Figure 1: Mean annual temperatures in France and Morocco from 1901 to 2015.

Country	France			Morocco		
Kernel	$K^{(0)}$	$K^{(1)}$	$K^{(2)}$	$K^{(0)}$	$K^{(1)}$	$K^{(2)}$
$MSPE$	0.3301302	2.090779	5.21788	0.7727975	5.110724	11.70042
$MAXPE$	1.3961	3.344106	5.312125	2.251341	6.171007	9.438383
Statistically	$K^{(0)}$ with 0.8198198 for $K^{(1)}$ and 0.8288288 for $K^{(2)}$			$K^{(0)}$ with 0.8288288 for $K^{(1)}$ and 0.8468468 for $K^{(2)}$		

Table 1: The three kernel selection criteria for the kernels $K^{(0)}$, $K^{(1)}$, $K^{(2)}$ using Morocco and France data.

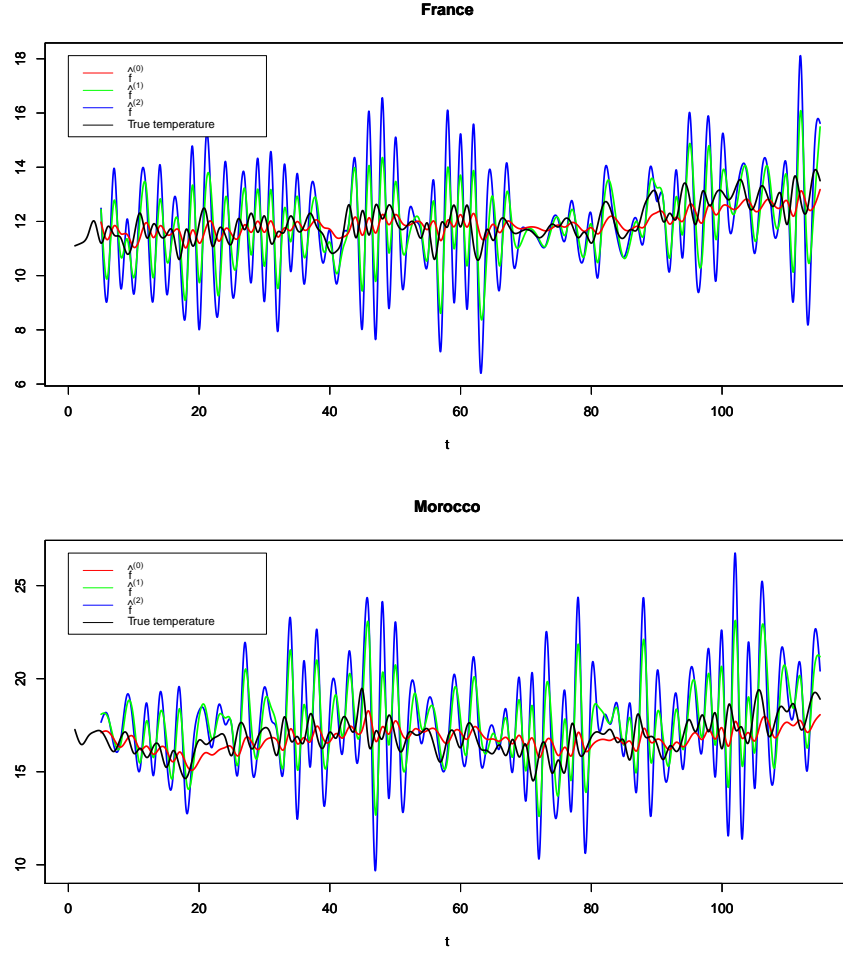


Figure 2: The splines of the predictors $\hat{f}^{(0)}$, $\hat{f}^{(1)}$, $\hat{f}^{(2)}$ and the true temperature.

Country	France			Morocco		
Kernel	$\mathbf{K}^{(0)}$	$\mathbf{K}^{(1)}$	$\mathbf{K}^{(2)}$	$\mathbf{K}^{(0)}$	$\mathbf{K}^{(1)}$	$\mathbf{K}^{(2)}$
Prediction	13.17656	15.48813	15.61992	18.06526	21.18307	20.41619
True temperature	13.5			18.9008		

Table 2: The predictors $\hat{f}^{(i)}(t_n)$, $n = 114$ (the mean annual temperature of the year 2015).

Country	France			Morocco		
Kernel	$\mathbf{K}^{(0)}$	$\mathbf{K}^{(1)}$	$\mathbf{K}^{(2)}$	$\mathbf{K}^{(0)}$	$\mathbf{K}^{(1)}$	$\mathbf{K}^{(2)}$
Prediction	12.91553	12.54049	11.40698	17.86737	18.99740	18.49113

Table 3: The predictors $\hat{f}^{(i)}(t_{n+1})$, $n = 114$ (the mean annual temperature of the year 2016).

Remark 5.1. Table 1 shows that the kernel $\mathbf{K}^{(0)}$ wins against $\mathbf{K}^{(1)}$ and $\mathbf{K}^{(2)}$ with respect to the three kernel selection criteria.

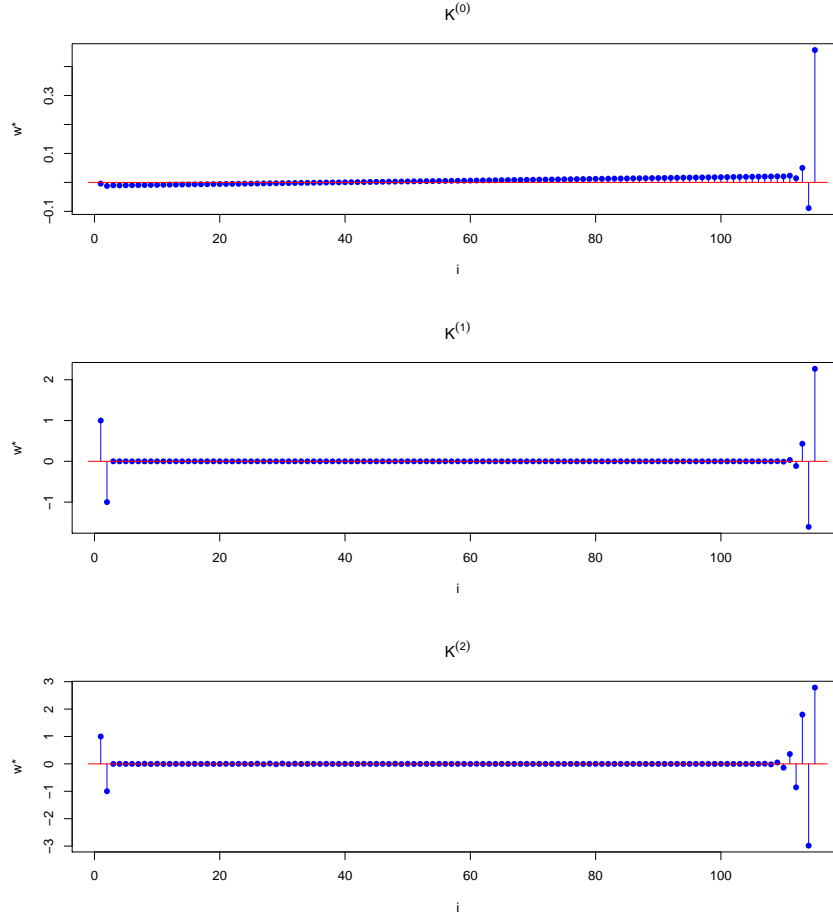


Figure 3: The w_1^*, \dots, w_n^* of (12) for the kernels $\mathbf{K}^{(0)}$, $\mathbf{K}^{(1)}$, $\mathbf{K}^{(2)}$.

5.3 Concluding remarks

The numerical results shows the three kernel selection criteria are stable, from Table 1 we have that the best kernel among the three kernels is $\mathbf{K}^{(0)}$ w.r.t. all the three criteria for both France and Morocco data. Moreover, the representation of the splines (Figure 2) shows that too.

From Table 1 and Figure 2 we have that the kernel $\mathbf{K}^{(1)}$ wins against $\mathbf{K}^{(2)}$. Considering the second derivative (u_2, \dots, u_n) as Gaussian with the covariance matrix Q^{-1} is a good stochastic modelization, at least is better than the assumption that (u_2, \dots, u_n) as Gaussian with the covariance matrix Q . Equivalently measuring the worst error in the unit ball using the norm $\|Q^{1/2}\mathbf{u}\|$ is better than the norm $\|Q^{-1/2}\mathbf{u}\|$.

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