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A NEW METHOD FOR SMOOTHING AND INTERPOLATING WITH INEQUALITY CONSTRAINTS

X. BAY[†], L. GRAMMONT[‡], AND H. MAATOUK^{†*}

Abstract. In this paper, smoothing curve or surface with both interpolation conditions and inequality constraints is considered as a general convex optimization problem in a Hilbert space. We propose a new approximation method based on a discretized optimization problem in a finite-dimensional Hilbert space under the same set of constraints. We prove that the approximate solution converges uniformly to the optimal constrained interpolating function. An efficient algorithm is derived and numerical examples with bound and monotonicity constraints in one and two dimensions are given. A comparison with existing monotone cubic splines interpolation algorithms in terms of linearized energy criterion is included.

Key words. RKHS, interpolation, smoothing, inequality constraints, splines

AMS subject classifications. 65D10, 65D07, 65D05, 47N10

1. Introduction. Let X be a nonempty set of \mathbb{R}^d ($d \geq 1$) and $E = \mathcal{C}^0(X)$ the linear (topological) space of real valued continuous functions on X . Given n distinct points $x^{(1)}, \dots, x^{(n)} \in X$ and $y_1, \dots, y_n \in \mathbb{R}$, we define the set I of interpolating functions by

$$I := \left\{ f \in E, f(x^{(i)}) = y_i, i = 1, \dots, n \right\}.$$

Let C be a closed convex set of E . We consider the following smoothing problem

$$(P) \quad \min \{ \|h\|_H^2, h \in H \cap C \cap I \}$$

where H is a Reproducing Kernel Hilbert Space (RKHS) continuously included in E . Notice that $H \cap C \cap I$ is a closed convex subset of H and the (unique) solution of (P) is the projection in H of the null function onto this convex set (assumed to be nonempty). The reproducing kernel (r.k.) K of H is a continuous symmetric definite-positive function:

$$K : (x, y) \in \mathbb{R}^d \times \mathbb{R}^d \longrightarrow K(x, y) := (K(., y), K(., x))_H \in \mathbb{R}.$$

Choosing different kernels, the norm with corresponding RKHS defines different notions of smoothness or different regularization criteria for scattered data interpolation.

In terms of the reproducing property (see [3]), the interpolation conditions can be formulated in the Hilbert space H as

$$(1.1) \quad \forall h \in H, \quad h(x^{(i)}) = (h, K(., x^{(i)}))_H = y_i, \quad i = 1, \dots, n.$$

Very often in practice, the convex set C is an infinite set of linear inequality constraints. The following smoothing interpolation problem without such constraints (case $C = E$)

$$(Q) \quad \min \{ \|h\|_H^2, h \in H \cap I \}$$

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has been solved so far. It is easy to prove that, if $H \cap I \neq \emptyset$, then (Q) has a unique solution. Let \mathcal{I} be the interpolation operator from H into \mathbb{R}^n defined as

$$\mathcal{I}(h) := \left(h(x^{(1)}), \dots, h(x^{(n)}) \right).$$

From equation (1.1), \mathcal{I} is a bounded linear operator whose range is included in the usual Euclidian space \mathbb{R}^n . The kernel $\text{Ker}(\mathcal{I})$ of \mathcal{I} is closed in H so that, for any $y \in \mathbb{R}^n$, $\check{h} = \mathcal{I}^\dagger(y)$ is the unique solution of (Q) , where \mathcal{I}^\dagger is the generalized inverse or Moore-Penrose inverse of \mathcal{I} (see [21]). If the matrix $\mathbb{K} = (K(x^{(i)}, x^{(j)}))_{1 \leq i, j \leq n}$ is invertible, $\check{h} = \mathcal{I}^\dagger(y)$ can be expressed as (see Proposition 2.3, §2.1)

$$(1.2) \quad \check{h}(x) = \mathbf{k}(x)^\top \mathbb{K}^{-1} \mathbf{y},$$

where $\mathbf{k}(x) = (K(x, x^{(1)}), \dots, K(x, x^{(n)}))^\top$ and $\mathbf{y} = (y_1, \dots, y_n)^\top$.

In many applications from science to engineering, there is a priori information on the shape of the solution such as lower and upper bounds or monotonicity property. The shape constraints restrict the reconstruction to some closed convex subset of the relevant function space. The general approach is based on using a minimization principle: the so called smoothing spline principle (see [2], [24]). The starting point is a characterization of the solution of the problem (P) as the orthogonal projection onto the convex set C of a finite linear combination (with unknown coefficients) of certain basis functions. The coefficients are defined from interpolation conditions which lead to a set of nonlinear equations that can be solved by Newton's method (see [2]).

If $\widehat{H \cap C} \cap \mathcal{I}^{-1}(\{\mathbf{y}\}) \neq \emptyset$ then (P) has a unique solution of the form

$$\hat{h} = P_C(\mathcal{I}^*(\alpha)) = P_C \left(\sum_{i=1}^n \alpha_i K(\cdot, x^{(i)}) \right),$$

where $\alpha = (\alpha_1, \dots, \alpha_n)^\top$ is a vector in \mathbb{R}^n and P_C is the orthogonal projection onto the convex set $H \cap C$ (see [20], Theorem 3.2, pp 739). Conversely, if for arbitrary vector α , $\hat{h} = P_C(\sum_i \alpha_i K(\cdot, x^{(i)}))$ satisfies the condition $\mathcal{I}(\hat{h}) = \mathbf{y}$ then \hat{h} is the solution of (P) (see [2], Theorem 2.1, pp 304). Under particular assumptions (see [20]), if $\hat{\alpha}$ is solution of the following dual problem

$$\min \left\{ \frac{1}{2} \|P_C(\mathcal{I}^*(\alpha))\|_H^2 - (\alpha, \mathbf{y}), \alpha \in \mathbb{R}^n \right\},$$

then $\hat{h} = P_C(\mathcal{I}^*(\hat{\alpha}))$ is the solution of (P) . In the general case (see [20], Theorem 3.2), $\hat{\alpha}$ is the solution the following dual problem

$$\min \left\{ \frac{1}{2} \|\mathcal{I}^*(\alpha)\|_H^2 - \frac{1}{2} \|\mathcal{I}^*(\alpha) - P_C(\mathcal{I}^*(\alpha))\|_H^2 - (\alpha, \mathbf{y}), \alpha \in \mathbb{R}^n \right\}.$$

This last problem is not easy to solve. As Andersson and Elfving wrote it in their paper [2], to transform this result into a numerical algorithm, it is necessary to compute the orthogonal projection P_C and the difficulty lies in that calculation. Andersson and Elfving [2] investigate the structure of the projection operator P_C for particular constraints defining the convex set C . Laurent [17] proposed an algorithm to solve this kind of minimization problem. This algorithm was applied by Utreras

and Varas in [23] for the K-Monotone Thin Plate Spline (K-M.T.P.S). The algorithm is based on iterations using Kuhn and Tucker's theorem. Moreover, as the authors wrote it in the paper [23], the computational cost of the dual-type algorithm is still high.

In this paper, we propose a new method to solve (P) . It is intended to overcome the computational cost problem and to be easy to implement. The philosophy is quite different from the methods constructed so far : it does not rely on minimization principles. We defined a discretized optimization problem (P_N) in a finite-dimensional space H_N under the same interpolation conditions and inequality constraints:

$$(P_N) \quad \min \{ \|h\|_{H_N}^2, h \in H_N \cap C \cap I \}$$

The main step of the method is the construction of the finite-dimensional Hilbert space H_N in the bigger space $E = \mathcal{C}^0(X)$, using a much more flexible set of basis functions in E to incorporate inequality constraints. In a particular framework, we prove that the problems (P) and (P_N) have a unique solution and that the solution of the discretized problem (P_N) tends to the solution of (P) , for the convergence in the space E (uniform convergence).

The article is organized as follows: in §2, the new method to approximate (P) is described and its convergence property is proved. In order to investigate the efficiency of the proposed approach, some numerical examples with bound and monotonicity constraints in one and two dimensions are given in §3. The algorithm is applied to classic spline cases with inequality constraints. In that case, a comparison with existing algorithms is included in §4.

2. A new algorithm based on a discretized optimization problem. Consider the infinite-dimensional convex optimization problem

$$(O) \quad \min \{ J(h), h \in H \cap C \},$$

where J is a real valued criterion defined on a Hilbert space H and C is a closed convex set of H .

By analogy with Finite Element Method (see the Ritz-Galerkin method [11]), a discretized optimization problem is of the form

$$(O_N) \quad \min \{ J(\rho_N h_N), h_N \in H_N \cap C_N \},$$

where $H_N = \pi_N(H)$ is a finite-dimensional space, π_N is a linear operator from H to H_N (projection or restriction operator), ρ_N is an extension operator from H_N to H and $C_N := \{ h_N \in H_N \text{ s.t. } \rho_N(h_N) \in C \}$ (see [5] and [18]). If $\pi_N(C) \subset C_N$ and under some stability and consistency properties of π_N and ρ_N , one can expect that $J(u_N) \rightarrow J(u)$ and $u_N \rightharpoonup u$ weakly in H , where u is the solution of (O) and u_N is the solution of (O_N) .

Our approach is different: we do not discretize the constraints set but we discretize the criterion:

$$\min \{ J_N(h_N), h_N \in H_N \cap C \}.$$

Nevertheless, the analysis of this discretized optimization problem involves a triple (H_N, π_N, ρ_N) , where π_N is a linear operator from E to $H_N \subset E$ and ρ_N is an operator from H_N to H . In this section, the space $E = \mathcal{C}^0(X)$ is the Banach space of continuous functions equipped with the uniform norm $\|\cdot\|_\infty$, where X is a compact subspace of \mathbb{R}^d . Let \hat{h} be the solution of (P) and \hat{h}_N the solution of (P_N) , we will prove that

$$\hat{h}_N \xrightarrow{N \rightarrow +\infty} \hat{h} \text{ in the space } E.$$

2.1. The approximating subspaces H_N and operators π_N and ρ_N . For simplicity, X is assumed to be the unit interval $[0, 1]$. Let Δ_N be a subdivision of $[0, 1]$ being a graded mesh:

$$\Delta_N : 0 = t_{N,0} < t_{N,1} < \dots < t_{N,N} = 1, \quad \Delta_N \subset \Delta_{N+1},$$

and $h_N = \max\{|t_{N,i+1} - t_{N,i}|, i = 0, \dots, N-1\} \xrightarrow{N \rightarrow +\infty} 0$. For each N , we define the approximating subspace H_N of $E = \mathcal{C}^0(X)$ to be the subspace of piecewise linear continuous functions associated to Δ_N . The canonical basis of H_N is formed by the so-called hat functions $[\varphi_{N,0}, \dots, \varphi_{N,N}]$:

$$(2.1) \quad j = 1, \dots, N-1 \quad \varphi_{N,j}(t) := \begin{cases} \frac{t - t_{N,j-1}}{t_{N,j} - t_{N,j-1}}, & t \in [t_{N,j-1}, t_{N,j}], \\ \frac{t_{N,j+1} - t}{t_{N,j+1} - t_{N,j}}, & t \in [t_{N,j}, t_{N,j+1}], \\ 0 & \text{otherwise.} \end{cases}$$

$$\varphi_{N,0}(t) := \begin{cases} \frac{t_{N,1} - t}{t_{N,1} - t_{N,0}}, & t \in [t_{N,0}, t_{N,1}], \\ 0 & \text{otherwise,} \end{cases} \quad \varphi_{N,N}(t) := \begin{cases} \frac{t - t_{N,N-1}}{t_{N,N} - t_{N,N-1}}, & t \in [t_{N,N-1}, t_{N,N}], \\ 0 & \text{otherwise.} \end{cases}$$

Next, we define the linear operators $\pi_N : E \rightarrow H_N$, $\rho_N : H_N \rightarrow H$ and a norm $\|\cdot\|_{H_N}$ such that π_N and ρ_N are stable, i.e.

$$\begin{aligned} \forall h \in H, \quad & \|\pi_N(h)\|_{H_N} \leq \|h\|_H, \\ \forall h_N \in H_N, \quad & \|\rho_N(h_N)\|_H \leq \|h_N\|_{H_N}, \end{aligned}$$

and π_N and ρ_N are consistent, i.e.

$$\forall h \in H, \quad \rho_N \circ \pi_N(h) \xrightarrow{N \rightarrow +\infty} h.$$

PROPOSITION 2.1. *Let π_N be the linear operator defined from E onto H_N by*

$$\forall f \in E, \quad \pi_N(f) = \sum_{j=0}^N f(t_{N,j}) \varphi_{N,j}.$$

Then, $\pi_N \circ \pi_N = \pi_N$ and

$$\pi_N(f) \xrightarrow{N \rightarrow +\infty} f \text{ in } E.$$

Proof. It is a classical result related to the usual Schauder basis of the Banach E (see [19]). \square

REMARK 2.2. Take $J(h) = \|h\|_H^2$ in (O). If $\|\rho_N h_N\|_H = \|h_N\|_{H_N}$, then (O_N) becomes a finite-dimensional problem easy to handle. So, it would be nice to construct the operator ρ_N and the norm on H_N satisfying this last equality.

For this, we consider the interpolation operator $\mathcal{I}_N : H \rightarrow \mathbb{R}^{N+1}$ by $\mathcal{I}_N(h) := (h(t_{N,0}), \dots, h(t_{N,N}))$. By the reproducing property, we also have

$$(2.2) \quad \mathcal{I}_N(h) = ((h, K(\cdot, t_{N,0}))_H, \dots, (h, K(\cdot, t_{N,N}))_H).$$

Hence, \mathcal{I}_N is a bounded operator and for all $y \in \mathbb{R}^{N+1}$, the following optimization problem

$$\min_{h \in H} \{ \|h\|_H^2, h(t_{N,j}) = y_j, j = 0, \dots, N \}$$

has a unique solution $\tilde{h} = \mathcal{I}_N^\dagger(y)$. Let us define the operator $\rho_N : H_N \rightarrow H$ as follows :

$$\forall h_N \in H_N, \quad \rho_N(h_N) = \mathcal{I}_N^\dagger(c_{h_N}),$$

where $c_{h_N} := (h_N(t_{N,0}), \dots, h_N(t_{N,N}))^\top$.

We assume in the following that the Gram matrix $\Gamma_N := (K(t_{N,i}, t_{N,j}))_{0 \leq i, j \leq N}$ is invertible for all N .

PROPOSITION 2.3. For all $h_N \in H_N$, we have

$$(2.3) \quad \rho_N(h_N) = \mathbf{k}(\cdot)^\top \Gamma_N^{-1} c_{h_N},$$

where $\mathbf{k}(\cdot) = (K(\cdot, t_{N,0}), \dots, K(\cdot, t_{N,N}))^\top$. Moreover,

$$(2.4) \quad \|\rho_N(h_N)\|_H^2 = c_{h_N}^\top \Gamma_N^{-1} c_{h_N}.$$

Proof. By definition, $\rho_N(h_N) \in \text{Ker}(\mathcal{I}_N)^\perp$. Additionally, from relation (2.2), we obtain

$$\text{Ker}(\mathcal{I}_N)^\perp = \text{span}(K(\cdot, t_{N,0}), \dots, K(\cdot, t_{N,N})),$$

so we can write for some α_j :

$$(2.5) \quad \rho_N(h_N) = \sum_{j=0}^N \alpha_j K(\cdot, t_{N,j}).$$

As $\rho_N(h_N)(t_{N,i}) = h_N(t_{N,i})$ for $i = 0, \dots, N$, we have $\alpha := (\alpha_0, \dots, \alpha_N)^\top = \Gamma_N^{-1} c_{h_N}$, which leads to equation (2.3). Using equation (2.5), one gets

$$\|\rho_N(h_N)\|_H^2 = (\rho_N(h_N), \rho_N(h_N))_H = \sum_{i=0}^N \sum_{j=0}^N \alpha_j \alpha_i (K(\cdot, t_{N,i}) K(\cdot, t_{N,j}))_H.$$

Since $(K(., t_{N,i}), K(., t_{N,j}))_H = K(t_{N,i}, t_{N,j})$, we obtain

$$\|\rho_N(h_N)\|_H^2 = \sum_{i=0}^N \sum_{j=0}^N \alpha_j \alpha_i K(t_{N,i}, t_{N,j}) = \alpha^\top \Gamma_N \alpha,$$

with $\alpha = \Gamma_N^{-1} c_{h_N}$, which completes the proof of the proposition. \square

In view of Proposition 2.3, let us construct an inner product in H_N so that $\|\rho_N(h_N)\|_H = \|h_N\|_{H_N}$.

THEOREM 2.4. *Define the scalar product in H_N by*

$$(2.6) \quad (f, g)_{H_N} := c_f^\top \Gamma_N^{-1} c_g,$$

with $c_f := (f(t_{N,0}), \dots, f(t_{N,N}))^\top$ and $c_g := (g(t_{N,0}), \dots, g(t_{N,N}))^\top$. Then, the space H_N is a RKHS with r.k. K_N given by

$$\forall x', x \in [0, 1], \quad K_N(x', x) = \sum_{i,j=0}^N K(t_{N,i}, t_{N,j}) \varphi_{N,j}(x) \varphi_{N,i}(x').$$

Proof. Clearly, H_N is a finite-dimensional Hilbert space. Let x be in $[0, 1]$. We have

$$(2.7) \quad K_N(., x) = \sum_{j=0}^N \lambda_{j,x} \varphi_{N,j} \in H_N,$$

where $\lambda_{j,x} = \sum_{k=0}^N K(t_{N,j}, t_{N,k}) \varphi_{N,k}(x) = (\Gamma_N \varphi(x))_j$, with $\varphi(x) := (\varphi_{N,0}(x), \dots, \varphi_{N,N}(x))^\top$.

Let $h := \sum_{i=0}^N \alpha_i \varphi_{N,i} \in H_N$. Using equation (2.6), we obtain

$$(h, K_N(., x))_{H_N} = \alpha^\top \Gamma_N^{-1} (\Gamma_N \varphi(x)) = \alpha^\top \varphi(x) = h(x),$$

which is the reproducing property in H_N . \square

PROPOSITION 2.5. *The operator ρ_N is stable. Indeed, ρ_N is an isometry from H_N into H , i.e.*

$$\forall h_N \in H_N, \quad \|\rho_N(h_N)\|_H^2 = \|h_N\|_{H_N}^2.$$

Furthermore,

$$(2.8) \quad \forall x \in X, \quad \rho_N(K_N(., x)) = \sum_{j=0}^N \varphi_{N,j}(x) K(., t_{N,j}).$$

Proof. Let h_N be in H_N , then $h_N = c_{h_N}^\top \varphi(x)$. According to the definition of the inner product in H_N , we have

$$\|h_N\|_{H_N}^2 = (h_N, h_N)_{H_N} = c_{h_N}^\top \Gamma_N^{-1} c_{h_N}.$$

Using (2.4), we obtain $\|\rho_N(h_N)\|_H^2 = \|h_N\|_{H_N}^2$. Since $c_{K_N(\cdot, x)} = \Gamma_N \varphi(x)$ (see equation (2.7)), we deduce the relation (2.8) from Proposition 2.3 and equation (2.3). \square

PROPOSITION 2.6. *For all f in E ,*

$$\|\pi_N(f)\|_{H_N}^2 = c_f^\top \Gamma_N^{-1} c_f,$$

with $c_f = (f(t_{N,0}), \dots, f(t_{N,N}))^\top$. Moreover, π_N is stable, i.e.

$$\forall h \in H, \quad \|\pi_N(h)\|_{H_N} \leq \|h\|_H.$$

Proof. The first part is a direct consequence of Theorem 2.4. Now, consider the orthogonal decomposition in H : $H = H_0^N \oplus H_1^N$, with

$$\begin{aligned} H_0^N &= \{h \in H : h(t_{N,j}) = 0, j = 0, \dots, N\}, \\ H_1^N &= \text{span}\{K(\cdot, t_{N,j}), j = 0, \dots, N\}. \end{aligned}$$

For all $h \in H$, there exists a unique $h_0 \in H_0^N$ and $h_1 \in H_1^N$ such that $h = h_0 + h_1$. Thus,

$$\|h_1\|_H^2 \leq \|h\|_H^2.$$

Additionally, every $h_1 \in H_1^N$ can be expressed as $h_1(\cdot) = \sum_{j=0}^N \alpha_j K(\cdot, t_{N,j})$. From the reproducing property $(K(\cdot, t_{N,j}), K(\cdot, t_{N,i}))_H = K(t_{N,i}, t_{N,j})$, we get

$$\|h_1\|_H^2 = (h_1, h_1)_H = \sum_{i,j=0}^N \alpha_i \alpha_j K(t_{N,i}, t_{N,j}) = \alpha^\top \Gamma_N \alpha.$$

As $h_1(t_{N,i}) = \sum_{j=0}^N \alpha_j K(t_{N,i}, t_{N,j})$ for $i = 0, \dots, N$, we have $\alpha = \Gamma_N^{-1} c_{h_1}$ and

$$\|h_1\|_H^2 = c_{h_1}^\top \Gamma_N^{-1} \Gamma_N \Gamma_N^{-1} c_{h_1} = c_{h_1}^\top \Gamma_N^{-1} c_{h_1}.$$

Since $h_0 \in H_0^N$, $c_{h_1} = c_h$ and $\|h_1\|_H^2 = c_h^\top \Gamma_N^{-1} c_h = \|\pi_N(h)\|_{H_N}^2$, which completes the proof of the proposition. \square

PROPOSITION 2.7. *Let Q_N be the orthogonal projection from H onto $(H_0^N)^\perp = H_1^N$. For all $h \in H$, we have*

$$\rho_N \circ \pi_N(h) = Q_N(h).$$

Moreover, (H_N, π_N, ρ_N) is consistent, i.e.

$$\rho_N(\pi_N(h)) \xrightarrow{N \rightarrow +\infty} h \text{ in } H.$$

Proof. According to the proof of Proposition 2.6, we have $Q_N(h) = \mathbf{k}(\cdot)^\top \Gamma_N^{-1} c_h$. On the other hand, we know that $\rho_N(\pi_N(h)) = \mathbf{k}(\cdot)^\top \Gamma_N^{-1} c_h$ from Proposition 2.3. Hence, $\rho_N \circ \pi_N$ is the orthogonal projection from H into H_1^N . To complete the proof of the proposition, it is sufficient to show that the subspace $\cup_N H_1^N$ is dense in H . Let h be in $(\cup_N H_1^N)^\perp$. By the reproducing property, we have $h(t_{N,i}) = 0$, for all $N \in \mathbb{N}$ and $i = 0, \dots, N$. By continuity, $h = 0$ and $(\cup_N H_1^N)^\perp = \{0\}$. \square

2.2. Existence and uniqueness of the solution of (P_N) . We recall the problems (P) , (P_N) respectively:

$$\min\{\|h\|_H^2, h \in H \cap C \cap I\} \quad \text{and} \quad \min\{\|h\|_{H_N}^2, h \in H_N \cap C \cap I\}.$$

Assumptions.

$$(H1) \quad \widehat{H \cap C} \cap I \neq \emptyset$$

$$(H2) \quad \forall N, \pi_N(C) \subset C$$

By the first hypothesis, the closed convex set $H \cap C \cap I$ is nonempty, so the initial problem (P) admits a unique solution \hat{h} .

Now, if $g \in \widehat{H \cap C} \cap I \neq \emptyset$, we will construct a sequence $g_N \in H \cap C$ such that $\lim_{N \rightarrow +\infty} g_N = g$ in H and $\pi_N(g_N) \in I$. Using $(H2)$ and also $(H1)$, this result will prove that $\pi_N(g_N)$ is in $H_N \cap C \cap I$ for N large enough. Thus, the problem (P_N) also admits a unique solution.

Let us construct now the sequence $(g_N)_N$ associated to $g \in \widehat{H \cap C} \cap I$. If $x^{(k)}$ is a data point, let $[a_{N,k}, b_{N,k}]$ be the smallest interval of Δ_N containing $x^{(k)}$, then we can write $x^{(k)} = \lambda_{N,k} a_{N,k} + (1 - \lambda_{N,k}) b_{N,k}$, where $\lambda_{N,k} \in [0, 1]$. Now we define the set

$$F_N := \{h \in H : \lambda_{N,k} h(a_{N,k}) + (1 - \lambda_{N,k}) h(b_{N,k}) = y_k, \quad k = 1, \dots, n\}.$$

We consider the following optimization problem:

$$(R_N) \quad \min_{h \in F_N} \|h - g\|_H^2.$$

According to the classical projection theorem, the problem (R_N) has a unique solution denoted by g_N .

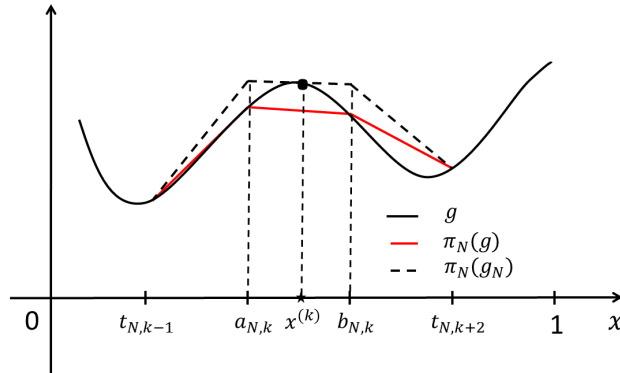


Fig. 1: The function $\pi_N(g_N)$ in the neighborhood of the data point $x^{(k)}$.

Figure 1 shows the projection $\pi_N(g_N)$ (black dashed line) of the solution of the problem (R_N) . Notice that the function $\pi_N(g)$ (red line) does not respect the interpolation condition.

LEMMA 2.8. *If $g \in \widehat{H \cap C} \cap I$, then $g_N \xrightarrow{N \rightarrow +\infty} g$ in H .*

Proof. We define the space G_0^N and G_1^N respectively as

$$\begin{aligned} G_0^N &:= \{h \in H : \lambda_{N,k}h(a_{N,k}) + (1 - \lambda_{N,k})h(b_{N,k}) = 0, \ k = 1, \dots, n\}, \\ G_1^N &:= \text{span} \{\lambda_{N,k}K(., a_{N,k}) + (1 - \lambda_{N,k})K(., b_{N,k}), \ k = 1, \dots, n\}. \end{aligned}$$

For arbitrary f in $F_N (\neq \emptyset)$, we have $F_N = f + G_0^N$ and $g_N = f + P_{G_0^N}(g - f)$, where $P_{G_0^N}$ is the orthogonal projection onto G_0^N . Therefore, $g - g_N = g - f - P_{G_0^N}(g - f) \in (G_0^N)^\perp = G_1^N$. Then, there exists $(\beta_1^N, \dots, \beta_n^N)^\top$ in \mathbb{R}^n such that

$$(2.9) \quad g - g_N = \sum_{k=1}^n \beta_k^N \epsilon_k^N,$$

where $\epsilon_k^N := \lambda_{N,k}K(., a_{N,k}) + (1 - \lambda_{N,k})K(., b_{N,k})$. The vector $\beta^N = (\beta_1^N, \dots, \beta_n^N)^\top$ can be seen as the solution of the following linear system

$$(2.10) \quad A^N \beta^N = \mathbf{b}^N,$$

where $A_{k,l}^N := (\epsilon_k^N, \epsilon_l^N)_H$ and $\mathbf{b}^N := (b_1^N, \dots, b_n^N)^\top$, with $b_k^N := \lambda_{N,k}g(a_{N,k}) + (1 - \lambda_{N,k})g(b_{N,k}) - y_k$. Now, each dot product

$$(\epsilon_k^N, \epsilon_l^N)_H = (\lambda_{N,k}K(., a_{N,k}) + (1 - \lambda_{N,k})K(., b_{N,k}), \lambda_{N,l}K(., a_{N,l}) + (1 - \lambda_{N,l})K(., b_{N,l}))_H$$

converges to $(K(., x^{(k)}), K(., x^{(l)}))_H = K(x^{(k)}, x^{(l)})$ by the continuity of $K(., .)$. On the other hand, the right vector in (2.10) converges to zero by continuity of the function g . Since the matrix $((K(., x^{(k)}), K(., x^{(l)}))_H)_{1 \leq k, l \leq n}$ is invertible, Lemma 2.8 is deduced from relations (2.9) and (2.10). \square

THEOREM 2.9. *Under the assumptions (H1) and (H2), the discretized optimization problem (P_N) has a unique solution \hat{h}_N (for N large enough).*

Proof. $H_N \cap C \cap I$ is a nonempty closed convex subset of H_N for N large enough. \square

2.3. Convergence analysis. LEMMA 2.10. *Let $h_1 \in H \cap C \cap I$ and $h_0 \in \widehat{H \cap C} \cap I$. Define $h_t := (1 - t)h_0 + th_1 \in H$, $t \in [0, 1]$. Then*

- h_t converges to h_1 when t tends to 1.
- $\forall t < 1$, $h_t \in \widehat{H \cap C} \cap I$.

Proof. The first property is straightforward. Now, since $h_0 \in \widehat{H \cap C}$, there exists $r > 0$ such that the open ball $B(h_0, r)$ is contained in $H \cap C$. For $t \in [0, 1]$, we define ϕ_t as:

$$\phi_t : h \in H \longrightarrow (1 - t)h_0 + th_1.$$

We have $\phi_t(H \cap C) \subset H \cap C$ so that $\phi_t(B(h_0, r)) = B(h_t, (1-t)r) \subset H \cap C$. Thus $h_t \in \widehat{H \cap C}^\circ$. The proof of the lemma is done since $h_0 \in I$, $h_1 \in I$ and I is convex. \square

LEMMA 2.11. *Let $\epsilon > 0$ be arbitrary small. There exists $g \in \widehat{H \cap C}^\circ \cap I$ such that $\|g\|_H \leq \|\hat{h}\|_H + \epsilon$, where \hat{h} is the solution of the problem (P).*

Proof. By assumption (H1), there exists $g \in \widehat{H \cap C}^\circ \cap I$. Using Lemma 2.10 with $h_0 = g$ and $h_1 = \hat{h} \in H \cap C \cap I$, we choose t such that $h_t \in \widehat{H \cap C}^\circ \cap I$ and $\|h_t - \hat{h}\|_H \leq \epsilon$, which implies that $\|h_t\|_H \leq \|\hat{h}\|_H + \epsilon$. \square

LEMMA 2.12. *Let $\epsilon > 0$. For N large enough, we have*

$$\|\hat{h}_N\|_{H_N} \leq \|\hat{h}\|_H + 2\epsilon.$$

Proof. Let $g \in \widehat{H \cap C}^\circ \cap I$ be such that $\|g\|_H \leq \|\hat{h}\|_H + \epsilon$ (see Lemma 2.11). Let g_N be the solution of (R_N) associated to g . By Lemma 2.8, we have for N large enough

$$\|g_N\|_H \leq \|g\|_H + \epsilon \leq \|\hat{h}\|_H + 2\epsilon.$$

Since $\pi_N(g_N) \in H_N \cap C \cap I$ and π_N is stable, we have $\|\hat{h}_N\|_{H_N} \leq \|\pi_N(g_N)\|_{H_N} \leq \|g_N\|_H$, which completes the proof of the lemma. \square

LEMMA 2.13. *For all x in X , $\rho_N(K_N(\cdot, x)) \xrightarrow{N \rightarrow +\infty} K(\cdot, x)$ in H . Furthermore,*

$$\sup_{x \in X} \|\rho_N(K_N(\cdot, x)) - K(\cdot, x)\|_H \xrightarrow{N \rightarrow +\infty} 0.$$

Proof. From Proposition 2.5, we have

$$\begin{aligned} \|\rho_N(K_N(\cdot, x)) - K(\cdot, x)\|_H^2 &= \|\rho_N(K_N(\cdot, x))\|_H^2 + \|K(\cdot, x)\|_H^2 - 2(\rho_N(K_N(\cdot, x)), K(\cdot, x))_H \\ &= \|K_N(\cdot, x)\|_{H_N}^2 + \|K(\cdot, x)\|_H^2 - 2 \sum_{j=0}^N \varphi_{N,j}(x) K(x, t_{N,j}) \\ &= K_N(x, x) + K(x, x) - 2 \sum_{j=0}^N \varphi_{N,j}(x) K(x, t_{N,j}). \end{aligned}$$

By uniform continuity of $K(\cdot, \cdot)$ on the compact set $X \times X$, we deduce that both $K_N(x, x) = \sum_{i,j=0}^N K(t_{N,i}, t_{N,j}) \varphi_{N,i}(x) \varphi_{N,j}(x)$ and $\sum_{j=0}^N \varphi_{N,j}(x) K(x, t_{N,j})$ are uniformly convergent to the function $K(x, x)$, which completes the proof of the lemma. \square

PROPOSITION 2.14. *Let \hat{h}_N and \hat{h} be respectively the solutions of (P_N) and (P) . Then*

1. $\|\hat{h}_N\|_{H_N}^2 \xrightarrow{N \rightarrow +\infty} \|\hat{h}\|_H^2$.
2. $\rho_N(\hat{h}_N) \xrightarrow{N \rightarrow +\infty} \hat{h}$ in H .

Proof. From Lemma 2.12, we have

$$\limsup_{N \rightarrow +\infty} \|\hat{h}_N\|_{H_N} \leq \|\hat{h}\|_H.$$

Additionally, by Proposition 2.5, $\|\rho_N(\hat{h}_N)\|_H = \|\hat{h}_N\|_{H_N}$, therefore $\limsup_{N \rightarrow +\infty} \|\rho_N(\hat{h}_N)\|_H \leq$

$\|\hat{h}\|_H < +\infty$. By weak compactness in Hilbert space, there exists a subsequence $(\rho_{N_k}(\hat{h}_{N_k}))_{k \in \mathbb{N}}$ which is weakly convergent:

$$(2.11) \quad \rho_{N_k}(\hat{h}_{N_k}) \xrightarrow{k \rightarrow +\infty} l \text{ in } H.$$

Let us prove that the limit function l is in $C \cap I$.

- $\forall k \in \mathbb{N}$ and $i = 1, \dots, n$

$$y_i = \hat{h}_{N_k}(x^{(i)}) = \left(\hat{h}_{N_k}, K_{N_k}(\cdot, x^{(i)}) \right)_{H_{N_k}} = \left(\rho_{N_k}(\hat{h}_{N_k}), \rho_{N_k}(K_{N_k}(\cdot, x^{(i)})) \right)_H.$$

Since $\rho_{N_k}(K_{N_k}(\cdot, x^{(i)})) \xrightarrow{k \rightarrow +\infty} K(\cdot, x^{(i)})$ strongly in H (see Lemma 2.13) and using (2.11), we have

$$\left(\rho_{N_k}(\hat{h}_{N_k}), \rho_{N_k}(K_{N_k}(\cdot, x^{(i)})) \right)_H \xrightarrow{k \rightarrow +\infty} (l, K(\cdot, x^{(i)}))_H = l(x^{(i)}),$$

which implies that $y_i = l(x^{(i)})$. Hence $l \in I$.

- Fix $N \geq 1$. We have $\pi_N(\hat{h}_{N_k}) \xrightarrow{k \rightarrow +\infty} \pi_N(l)$ in the finite-dimensional space H_N because $\hat{h}_{N_k}(t_{N,i}) \xrightarrow{k \rightarrow +\infty} l(t_{N,i})$ by the previous argument showing $l \in I$. Since $\hat{h}_{N_k} \in C$, $\pi_N(C) \subset C$ and $C \cap H_N$ is closed in H_N , we have $\pi_N(l) \in C$. As $\pi_N(l)$ converges to l in E (see Proposition 2.1) and C is closed for the topology of E , one gets $l \in C$.

Since $l \in H \cap C \cap I$, we have

$$\|\hat{h}\|_H^2 \leq \|l\|_H^2.$$

As $\rho_{N_k}(\hat{h}_{N_k}) \xrightarrow{k \rightarrow +\infty} l$ in H , we know that $\|l\|_H \leq \liminf_{k \rightarrow +\infty} \|\rho_{N_k}(\hat{h}_{N_k})\|_H$. So,

$$(2.12) \quad \limsup_{k \rightarrow +\infty} \|\rho_{N_k}(\hat{h}_{N_k})\|_H \leq \|\hat{h}\|_H \leq \|l\|_H \leq \liminf_{k \rightarrow +\infty} \|\rho_{N_k}(\hat{h}_{N_k})\|_H.$$

Hence, $\|l\|_H = \|\hat{h}\|_H$ and $l = \hat{h}$ by unicity of the solution of the problem (P) . From inequalities (2.12), we deduce that $\|\rho_{N_k}(\hat{h}_{N_k})\|_H \xrightarrow{k \rightarrow +\infty} \|\hat{h}\|_H$. But, weak convergence (see (2.11)) and convergence of the sequence of the norms imply strong convergence. Hence, the subsequence $\rho_{N_k}(\hat{h}_{N_k})$ converges strongly to \hat{h} and the sequence $(\rho_N(\hat{h}_N))_N$ as well. \square

The first part of Proposition 2.14 is a crucial step for convergence analysis of the sequence of the minimizers $(\hat{h}_N)_N$. The following theorem summarizes the main results of this paper.

THEOREM 2.15. *Under assumptions (H1) and (H2), the discretized optimization problem (P_N) has an unique solution $\hat{h}_N \in H_N \subset E = C^0(X)$ (for N large enough). Let \hat{h} be the unique solution in the RKHS $H \subset E$ of the constrained interpolation smoothing problem (P) . Then, we have*

$$\hat{h}_N \xrightarrow{N \rightarrow +\infty} \hat{h} \text{ in } E,$$

and

$$\begin{aligned} \|\hat{h}_N\|_{H_N}^2 &\xrightarrow{N \rightarrow +\infty} \|\hat{h}\|_H^2, \\ \rho_N(\hat{h}_N) &\xrightarrow{N \rightarrow +\infty} \hat{h} \text{ in } H. \end{aligned}$$

Proof. Let \hat{h} and \hat{h}_N be the solutions of (P) and (P_N) respectively. Then

$$\begin{aligned} \hat{h}_N(x) - \hat{h}(x) &= \left(\hat{h}_N, K_N(., x) \right)_{H_N} - \left(\hat{h}, K(., x) \right)_H \\ &= \left(\rho_N(\hat{h}_N), \rho_N(K_N(., x)) \right)_H - \left(\hat{h}, K(., x) \right)_H \\ &= \left(\rho_N(\hat{h}_N), \rho_N(K_N(., x)) - K(., x) \right)_H + \left(\rho_N(\hat{h}_N) - \hat{h}, K(., x) \right)_H. \end{aligned}$$

The proof of the theorem is done by applying Proposition 2.14 and Lemma 2.13 to the following inequality

$$\begin{aligned} \sup_{x \in X} |\hat{h}_N(x) - \hat{h}(x)| &\leq \|\rho_N(\hat{h}_N)\|_H \times \sup_{x \in X} \|\rho_N(K_N(., x)) - K(., x)\|_H \\ &\quad + \|\rho_N(\hat{h}_N) - \hat{h}\|_H \times \sup_{x \in X} \|K(., x)\|_H \end{aligned}$$

since $\sup_{x \in X} \|K(., x)\|_H = \sup_{x \in X} \sqrt{K(x, x)} < +\infty$ (K is a continuous function in X^2). \square

2.4. Implementation of (P_N) . The aim of this section is to show that the discretized optimization problem (P_N) is equivalent to a quadratic program (QP). To do this, we define the application ψ from \mathbb{R}^{N+1} to H_N as follows:

$$\psi : \alpha \in \mathbb{R}^{N+1} \longrightarrow \psi(\alpha) = \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j}(\cdot) \in H_N,$$

where $\varphi_{N,j}$, $j = 0, \dots, N$ are defined in (2.1). Define a new scalar product on \mathbb{R}^{N+1} as

$$(\alpha, \beta)_{\mathbb{R}^{N+1}} := \alpha^\top \Gamma_N^{-1} \beta$$

The application ψ is a norm preserving isomorphism. For all $f \in H_N$ such that $f(x) = \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j}(x)$, we have

$$\|f\|_{H_N}^2 = \alpha^\top \Gamma_N^{-1} \alpha = \|\alpha\|_{\mathbb{R}^{N+1}}^2.$$

Using the isomorphism ψ , we define the following closed convex subset of \mathbb{R}^{N+1} , $\tilde{C} := \psi^{-1}(C)$ and $\tilde{I} := \psi^{-1}(I)$ the following affine subspace of \mathbb{R}^{N+1} :

$$\tilde{I} = \left\{ \alpha \in \mathbb{R}^{N+1} \text{ such that } \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j}(x^{(i)}) = y_i, \ i = 1, \dots, n \right\}.$$

Consider now the QP problem

$$(\tilde{P}_N) \quad \arg \min_{\substack{\alpha \in \mathbb{R}^{N+1} \\ \alpha \in \tilde{I} \cap \tilde{C}}} \alpha^\top \Gamma_N^{-1} \alpha,$$

where \tilde{I} and \tilde{C} represent respectively the interpolation condition and the inequality constraints in the Euclidian space \mathbb{R}^{N+1} . The numerical calculation of (\tilde{P}_N) is a classical problem in the optimization of positive quadratic forms, see e.g. [4] and [12].

PROPOSITION 2.16. *The solution of the discretized optimization problem (P_N) is*

$$\hat{h}_N = \sum_{j=0}^N (\alpha_{opt})_j \varphi_{N,j},$$

where $\alpha_{opt} \in \mathbb{R}^{N+1}$ is the unique solution of problem (\tilde{P}_N) .

3. Numerical Illustration. This section is devoted to numerical examples to illustrate the approximation method in various situations.

3.1. Bound constraints. Let us recall that $E = \mathcal{C}^0([0,1])$. Let H be the RKHS whose reproducing kernel is the commonly used squared exponential (or Gaussian) kernel $K(x, y) = \exp\left(-\frac{(x-y)^2}{2\theta^2}\right)$, where the parameter θ defines a characteristic length-scale [22]. The norm on the induced RKHS defines a strong smoothness criterion for data interpolation. The set C of inequality constraints is of the form

$$C = \{f \in E : -\infty \leq a \leq f(x) \leq b \leq +\infty, \ x \in [0, 1]\},$$

where the lower and upper bounds a and b are assumed to be known. Notice that C is a closed convex set of E .

In the following proposition, we give a characterization of the functions in both H_N and C . This characterization is easy to use in practice.

PROPOSITION 3.1. *Let $h_N \in H_N$. Then,*

$$h_N := \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j} \in C \text{ if and only if the coefficients } \alpha_{N,j} \in [a, b], \ j = 0, \dots, N.$$

Proof. Observe that $\forall x \in [0, 1]$, $\sum_{j=0}^N \varphi_{N,j}(x) = 1$. Now if the coefficients $\alpha_{N,j}$ lie in the interval $[a, b]$, then h_N is in C . Conversely, if $h_N \in C$, then

$$h_N(t_{N,i}) = \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j}(t_{N,i}) = \sum_{j=0}^N \alpha_{N,j} \delta_{i,j} = \alpha_{N,i} \in [a, b],$$

which completes the proof of the proposition. \square

From Proposition 3.1, we immediately see that hypothesis (H2) holds, i.e. $\pi_N(C) \subset C$ for all N . Let \hat{h}_N be the solution of the finite optimization problem (P_N) . From Proposition 2.16 and Proposition 3.1, \hat{h}_N can be expressed as

$$x \in [0, 1], \quad \hat{h}_N(x) = \sum_{j=0}^N (\alpha_{opt})_j \varphi_{N,j}(x),$$

where $\alpha_{opt} \in \mathbb{R}^{N+1}$ is the solution of the following QP:

$$\arg \min_{\substack{\alpha \in \mathbb{R}^{N+1} \\ \alpha \in \tilde{I} \cap \tilde{C}}} \|\alpha\|_{\mathbb{R}^{N+1}}^2, \quad \text{where}$$

$$\tilde{I} = \left\{ \alpha \in \mathbb{R}^{N+1} : \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j}(x^{(i)}) = y_i, \quad i = 1, \dots, n \right\},$$

$$\tilde{C} = \left\{ \alpha \in \mathbb{R}^{N+1} : a \leq \alpha_{N,j} \leq b, \quad j = 0, \dots, N \right\}.$$

To ensure the hypothesis (H1), we need to suppose

$$a < y_i < b, \quad i = 1, \dots, n.$$

In the illustration example (see Figure 2), $a = 0$, $b = 1$ and $n = 6$. The value of the parameter θ is fixed to 0.18.

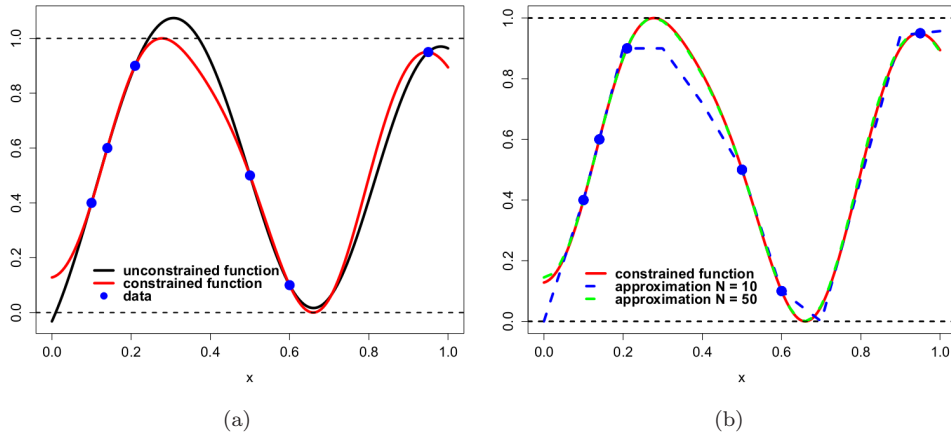


Fig. 2: Unconstrained and constrained interpolating function (\hat{h}_N with $N = 500$) (Figure 2a). Convergence of the discretized solution \hat{h}_N , $N = 10$ and $N = 50$ (Figure 2b).

In order to investigate the efficiency of the proposed method, we plot in Figure 2a the solution of problem (P) without bound constraints (equation (1.2), black line)

and the solution of the discretized optimization problem (P_N) \hat{h}_N for $N = 500$ (red line), which is assumed to be very closed to the function \hat{h} . Unlike the first solution, the last one respects both interpolation conditions and bound constraints. Figure 2b shows the convergence of the proposed approximate solution. The red line is the function \hat{h}_N for $N = 500$. The blue and the green dashed line represent respectively the function \hat{h}_N for $N = 10$ and $N = 50$.

3.2. Monotonicity in one dimension. E and H are the spaces defined in the previous §3.1. The convex set C is the space of monotone non-decreasing functions and is defined as

$$C := \{f \in \mathcal{C}^0([0, 1]) : f(x) \leq f(x') \text{ if } x \leq x'\}.$$

Using the notation introduced before, we have the following result:

PROPOSITION 3.2. *Let $h_N \in H_N$. Then, $h_N(x) := \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j}(x)$ is non-decreasing if and only if the sequence $(\alpha_{N,j})_{j=0,\dots,N}$ is non-decreasing (i.e. $\alpha_{j-1,N} \leq \alpha_{N,j}$, $j = 1, \dots, N$).*

Proof. If the sequence $(\alpha_{N,j})_{j=0,\dots,N}$ is non-decreasing then h_N is non-decreasing since h_N is a piecewise linear function. Conversely, the sequence $(\alpha_{N,j})_j = (h_N(t_{N,j}))_j$, $j = 0, \dots, N$ is a non-decreasing sequence. \square

From this proposition, we see again that hypothesis (H2) holds, i.e. $\pi_N(C) \subset C$ for all N . Moreover, the interpolation conditions and the inequality constraints in \mathbb{R}^{N+1} can be expressed as follow:

$$(3.1) \quad \tilde{I} = \left\{ \alpha \in \mathbb{R}^{N+1} : \sum_{j=0}^N \alpha_{N,j} \varphi_{N,j}(x^{(i)}) = y_i, \ i = 1, \dots, n \right\},$$

$$(3.2) \quad \tilde{C} = \{ \alpha \in \mathbb{R}^{N+1} : \alpha_{N,j-1} \leq \alpha_{N,j}, \ j = 0, \dots, N \}.$$

To ensure the hypothesis (H1), we suppose

$$y_{i-1} < y_i, \quad i = 2, \dots, n.$$

From Proposition 2.16, the solution of problem (P_N) is equal to

$$x \in [0, 1], \quad \hat{h}_N(x) = \sum_{j=0}^N (\alpha_{opt})_j \varphi_{N,j}(x),$$

where $\alpha_{opt} \in \mathbb{R}^{N+1}$ is the solution of the problem (\tilde{P}_N) , where \tilde{I} and \tilde{C} are defined in (3.1) and (3.2) respectively. Figure 3 shows the efficiency and the convergence of the proposed algorithm. In Figure 3a, the black line is the solution of problem (P) without monotonicity constraints and the red line is the solution of the discretized optimization problem (P_N) for $N = 500$. Notice that only the last one respects both interpolation conditions and monotonicity constraints. In Figure 3b, convergence of different approximations is illustrated. The red line represents the function \hat{h}_N for $N = 500$ and the blue line (resp. the green line) corresponds to the function \hat{h}_N for $N = 5$ (resp. $N = 20$).

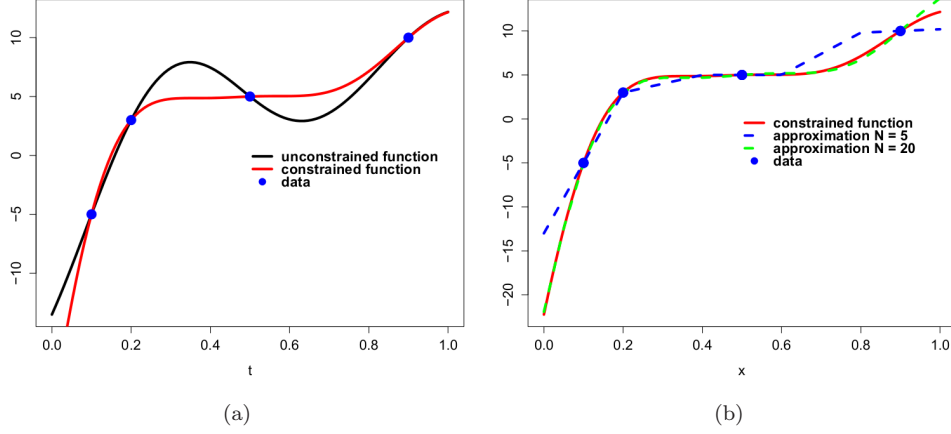


Fig. 3: Unconstrained and constrained interpolating function (\hat{h}_N with $N = 500$) (Figure 3a). Convergence of discretized solutions \hat{h}_N , $N = 5$ and $N = 20$ (Figure 3b).

3.3. Case of a finite number of constraints. The so-called *constrained* interpolation splines are defined as solutions of problem (P) where the general norm (semi-norm) is defined from a differential operator. In the framework of spline theory, the problem of interpolation under a finite number of inequality constraints has been solved (see e.g. [8], [9] in \mathbb{R}^2 and [16] in \mathbb{R}). Our aim in this section is only to assess the convergence of the proposed method by comparing it with the analytical solution. To do this, let us draw attention that our method can be easily applied to a finite number of inequality constraints. In the following, we will recall the main results given in [8]. Firstly, the interpolation conditions are defined as $f(x^{(i)}) = y_i$, $i = 1, \dots, n$. Secondly, the finite number of inequality constraints are denoted respectively lower and upper inequality constraints and are defined as in [8]:

$$(3.3) \quad f(x^{(i)}) \geq y_i, \quad i = n+1, \dots, n+p_1,$$

$$(3.4) \quad f(x^{(i)}) \leq y_i, \quad i = n+p_1+1, \dots, n+p_1+p_2.$$

In this case, we have n interpolation conditions and p inequality constraints with $p = p_1 + p_2$. The analytical form of the constrained interpolation spline is given by Dubrule and Kostov in [8]:

$$(3.5) \quad \sigma(x) = \sum_{i=1}^{n+p} b^i K(x, x^{(i)}),$$

where the function K is the underlying reproducing kernel of the RKHS H . The $(n+p)$ coefficients $b = (b^1, \dots, b^{n+p})^\top$ are obtained by solving the following quadratic optimization problem:

$$\arg \min_b \sum_{i=1}^{n+p} \sum_{j=1}^{n+p} b^i b^j K(x^{(i)}, x^{(j)}),$$

under the n interpolation conditions ($f(x^{(i)}) = y_i$, $i = 1, \dots, n$) and the p inequality constraints given in (3.3) and (3.4). This form is generalized to any kernel or semi-kernel, stationary covariance function or generalized covariance function, see [8] and [15].

The convex set C is the subset of functions that verify (3.3) and (3.4). In that case, the solution of the discretized optimization problem (P_N) is expressed as follows:

$$(3.6) \quad \hat{h}_N(x) = \sum_{j=0}^N (\alpha_{opt})_j \varphi_{N,j}(x)$$

where the $(N+1)$ coefficients $((\alpha_{opt})_0, \dots, (\alpha_{opt})_N)$ are the solution of the following quadratic optimization problem

$$\arg \min_{\substack{\alpha \in \mathbb{R}^{N+1} \\ \alpha \in \tilde{I} \cap \tilde{C}}} \|\alpha\|_{\mathbb{R}^{N+1}}^2, \quad \text{where}$$

$$\begin{aligned} \tilde{I} &= \left\{ \alpha \in \mathbb{R}^{N+1} \text{ such that } \hat{h}_N(x^{(i)}) = y_i, \ i = 1, \dots, n \right\}, \\ \tilde{C} &= \left\{ \alpha \in \mathbb{R}^{N+1} \text{ such that } \hat{h}_N \text{ verifies (3.3) and (3.4)} \right\}. \end{aligned}$$

In Figure 4, the kernel is the Matérn 3/2 covariance kernel defined as follows:

$$K_{m_{\frac{3}{2}}}(x, y) = \left(1 + \frac{\sqrt{3}|x - y|}{\theta} \right) \exp \left(-\frac{\sqrt{3}|x - y|}{\theta} \right),$$

where θ is a smoothing parameter of value 0.3. We choose $n = 6$ interpolation conditions and $p = 3$ inequality constraints ($p_1 = 2$ and $p_2 = 1$). The black line represents the constrained interpolation spline given by (3.5). In Figures 4a and 4b, we plot respectively the function \hat{h}_N given in (3.6) for $N = 10$ and $N = 40$. Notice that \hat{h}_N respects both interpolation conditions and inequality constraints and coincides with the constrained interpolation spline when N is large enough.

In Figure 5, the Gaussian kernel is used where the parameter θ is also equal to 0.3. The black line represents the constrained interpolation spline using Dubrule's algorithm. The red dashed line is the function \hat{h}_N defined as the solution of problem (P_N) for $N = 10$ (Figure 5a) and $N = 40$ (Figure 5b).

3.4. Monotonicity in multidimensional cases. Let us begin by the two dimensional case where $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$. The unknown function f is assumed to be continuous and monotone non-decreasing on the unit square $X = [0, 1] \times [0, 1]$:

$$x_1 \leq x'_1 \quad \text{and} \quad x_2 \leq x'_2 \quad \Rightarrow \quad f(x_1, x_2) \leq f(x'_1, x'_2).$$

Like the one dimensional case, we construct the basis functions such that the monotonicity constraints are *equivalent* to constraints on the coefficients. First, we discretize the unit square, e.g. uniformly with $(N+1)^2$ knots, see Figure 6 for $N = 7$. Then, the basis function at the knot $(t_{N,i}, t_{N,j})$ is defined as

$$\varphi_{i,j}(\mathbf{x}) := \varphi_{N,i}(x_1) \varphi_{N,j}(x_2),$$

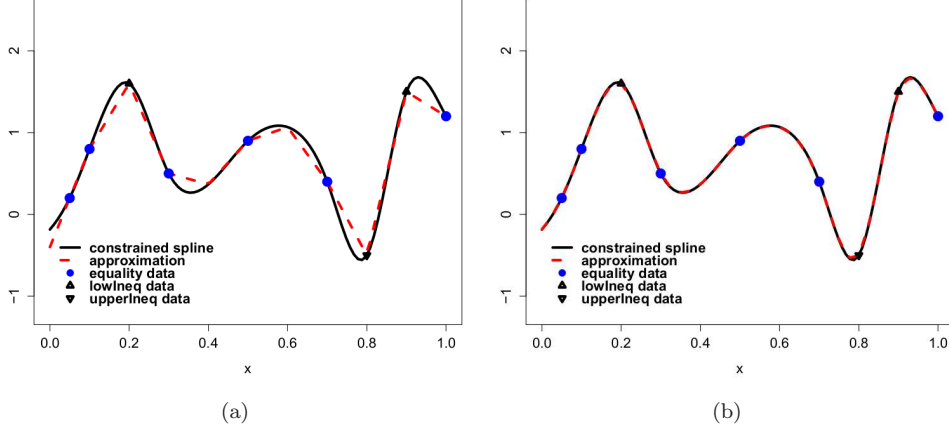


Fig. 4: The black line represents the constrained interpolation spline using the Matérn 3/2 kernel. The red dashed-line corresponds to the function \hat{h}_N for $N = 10$ (Figure 4a) and $N = 40$ (Figure 4b).

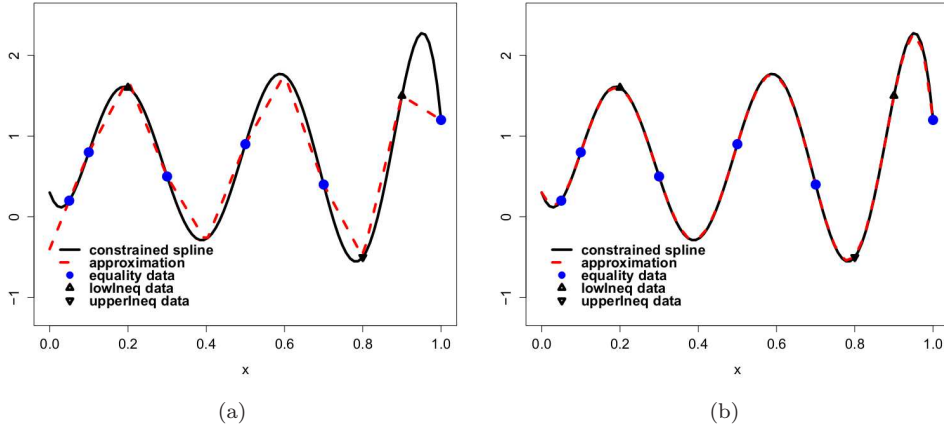


Fig. 5: The black line represents the constrained interpolation spline using the Gaussian kernel. The red dashed-line corresponds to the function \hat{h}_N for $N = 10$ (Figure 5a) and $N = 40$ (Figure 5b).

where $\varphi_{N,j}$, $j = 0, \dots, N$ are given in (2.1). Now, we have

$$\varphi_{i,j}(t_{N,k}, t_{N,l}) = \varphi_{N,i}(t_{N,k})\varphi_{N,j}(t_{N,l}) = \delta_{i,k}\delta_{j,l}, \quad k, l = 0, \dots, N.$$

PROPOSITION 3.3. *Let $h_N \in H_N$. Then, $h_N(\mathbf{x}) := \sum_{i,j=0}^N \alpha_{i,j} \varphi_{N,i}(x_1) \varphi_{N,j}(x_2)$ is non-decreasing with respect to the two input variables if and only if the $(N+1)^2$ coefficients $\alpha_{i,j}$, $i, j = 0, \dots, N$ verify the following linear constraints:*

$$(i) \quad \alpha_{i-1,j} \leq \alpha_{i,j} \text{ and } \alpha_{i,j-1} \leq \alpha_{i,j}, \quad i, j = 1, \dots, N$$

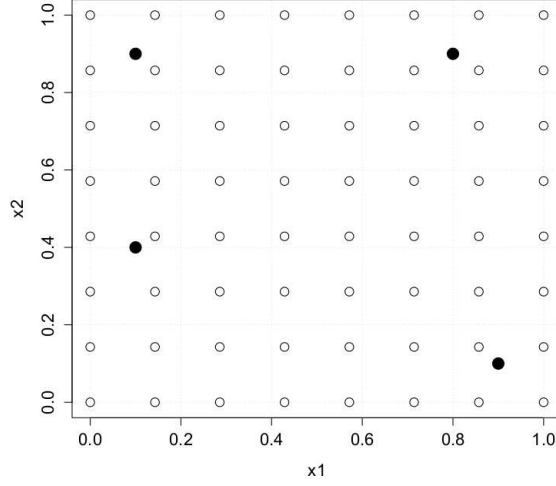


Fig. 6: Data for the monotone 2D interpolation problem (black points) and knots $(t_{N,i}, t_{N,j})_{0 \leq i,j \leq 7}$ used to define the basis functions.

- (ii) $\alpha_{i-1,0} \leq \alpha_{i,0}, \quad i = 1, \dots, N$
- (iii) $\alpha_{0,j-1} \leq \alpha_{0,j}, \quad j = 1, \dots, N$

Proof. If the $(N+1)^2$ coefficients $\alpha_{i,j}$, $i, j = 0, \dots, N$ verify the above linear constraints (i), (ii) and (iii), then h_N is non-decreasing as a piecewise linear function with respect to x_1 or x_2 direction. Conversely, the relations $h_N(t_{N,i}, t_{N,j}) = \alpha_{i,j}$, $i, j = 0, \dots, N$ complete the proof of the proposition. \square

Consequently and from Proposition 2.16, the solution of the problem (P_N) can be expressed as

$$\hat{h}_N(\mathbf{x}) = \sum_{i,j=0}^N (\alpha_{opt})_{i,j} \varphi_{N,i}(x_1) \varphi_{N,j}(x_2),$$

where $\alpha_{opt} = (\alpha_{opt})_{i,j}$ is the solution of the following QP:

$$\arg \min_{\substack{\alpha \in \mathbb{R}^{(N+1)^2} \\ \alpha \in \tilde{I} \cap \tilde{C}}} \|\alpha\|_{\mathbb{R}^{(N+1)^2}}^2,$$

with $\tilde{C} = \left\{ \alpha \in \mathbb{R}^{(N+1)^2} \text{ such that inequalities 1, 2 and 3 are satisfied in Proposition 3.3} \right\}$ and \tilde{I} is defined by (3.1).

In Figure 7, we take the kernel to be the 2-dimensional Gaussian kernel

$$K(x, y) = \exp\left(-\frac{(x_1 - y_1)^2}{2\theta_1^2}\right) \times \exp\left(-\frac{(x_2 - y_2)^2}{2\theta_2^2}\right)$$

with smoothing parameters $(\theta_1, \theta_2) = (0.4, 0.4)$. In Figures 7a and 7b, we plot respectively the solution of the discretized optimization problem (P_N) \hat{h}_N for $N = 20$ and the associated contour levels. Notice that \hat{h}_N satisfies both interpolation conditions and monotonicity (non-decreasing) constraints with respect to the two input variables. Figure 8 shows the case where the true function is known to be monotone (non-decreasing) for the second variable only (see Remark 3.4 below). In this case, the set of constraints is $C := \{f \in E : f(x_1, x_2) \leq f(x_1, x'_2), \text{ if } x_2 \leq x'_2\}$, where $E = \mathcal{C}^0(X)$.

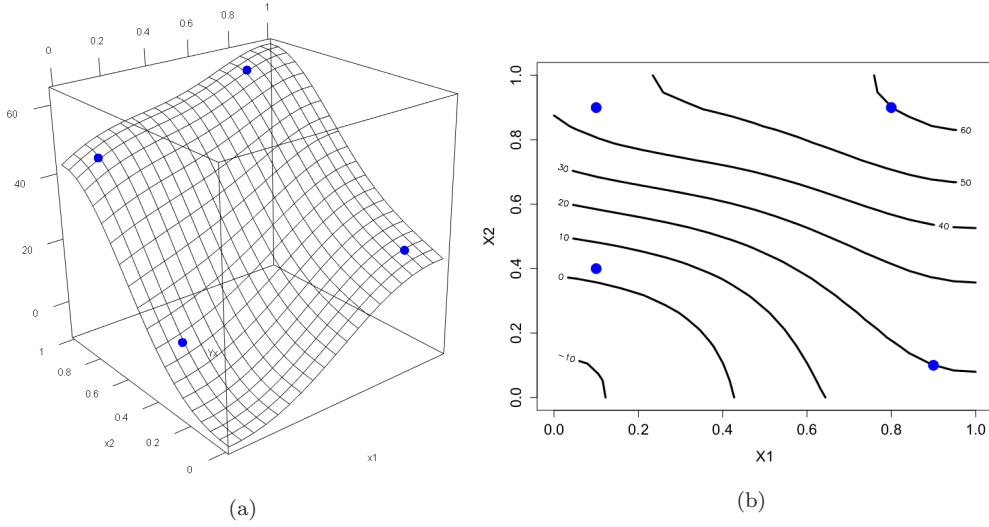


Fig. 7: The solution \hat{h}_N of the discretized optimization problem (P_N) (Figure 7a) and the associated contour levels (Figure 7b).

REMARK 3.4. *Proposition 3.3 can be easily extended to the monotonicity with respect to one of the input variables. For instance, the function h_N defined in Proposition 3.3 is non-decreasing with respect to the second variable if and only if the $(N+1)^2$ coefficients verify: $\alpha_{i,j-1} \leq \alpha_{i,j}$, $j = 1, \dots, N$ and $i = 0, \dots, N$.*

REMARK 3.5. *The monotonicity in the general multidimensional case is a simple extension of the two-dimensional case. Remark 3.4 can be extended as well for the monotonicity with respect to any subset of the variables x_1, \dots, x_d .*

4. Splines case. The aim of this section is to compare the method described in this paper with existing algorithms. We focus on cubic spline interpolation with inequality constraints.

4.1. Constrained Cubic Spline Interpolation. Cubic splines can be defined as functions minimizing the following well-known criterion (linearized energy (LE) measure, see e.g. [25]):

$$(4.1) \quad E_L = \int_0^1 (f''(t))^2 dt,$$

given the n observations (interpolation conditions) $f(x^{(i)}) = y_i$, $i = 1, \dots, n$. A cubic spline is known to be a third-order polynomial function f_k on each subinterval

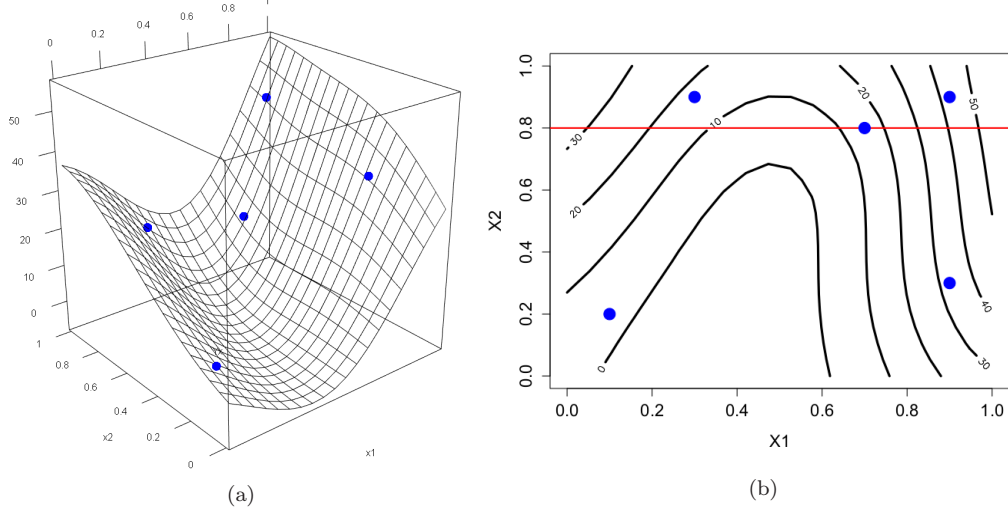


Fig. 8: The solution \hat{h}_N of the discretized optimization problem (P_N) using Remark 3.4 (Figure 8a) and the associated contour levels (Figure 8b).

$[x^{(k)}, x^{(k+1)}], (k = 1, \dots, n-1)$:

$$(4.2) \quad f_k(x) = a_k(x - x^{(k)})^3 + b_k(x - x^{(k)})^2 + c_k(x - x^{(k)})d_k,$$

where a_k, b_k, c_k, d_k are spline coefficients. It is also known to be linear on the first subinterval $[0, x^{(1)}]$ and the last subinterval $[x^{(n)}, 1]$. Thus, the LE measure criterion can be written in terms of spline coefficients as follows:

$$(4.3) \quad \begin{aligned} E_L &= \int_{x^{(1)}}^{x^{(n)}} (f''(x))^2 dx \\ &= \sum_{k=1}^{n-1} \int_{x^{(k)}}^{x^{(k+1)}} (f_k''(x))^2 dx = \sum_{k=1}^{n-1} \int_{x^{(k)}}^{x^{(k+1)}} (6a_k(x - x^{(k)}) + 2b_k)^2 dx \\ &= \sum_{k=1}^{n-1} 12a_k^2 \Delta x^{(k)}^3 + 12a_k b_k \Delta x^{(k)}^2 + 4b_k^2 \Delta x^{(k)}, \end{aligned}$$

where $\Delta x^{(k)} = x^{(k+1)} - x^{(k)}$.

With additional inequality constraints (such as bound, monotonicity or convexity constraints), the function minimizing the LE criterion is called a *constrained cubic spline*. In the case of monotonicity constraints, this type of problem has been studied so far (see e.g. [1], [10], [13] and [25]) and [7] for non-negativity, monotonicity and convexity constraints.

First, let us show how we can adapt our method to this important case. The problem (P) can be seen as

$$(4.4) \quad \min \left\{ \int_0^1 (h''(t))^2 dt, h \in H^2 \cap C \cap I \right\},$$

where H^2 is the Sobolev space $\{h \in L^2([0, 1]) \text{ such that } h', h'' \in L^2([0, 1])\}$, I and C are respectively the space of interpolation conditions and inequality constraints. Notice that H^2 is continuously embedded in the space $\mathcal{C}^1([0, 1])$ of continuously differentiable functions on $X = [0, 1]$. The LE criterion defines a semi-norm of kernel $\mathbb{R} \oplus \mathbb{R}x$. Now, H^2 can be decomposed as follows:

$$(4.5) \quad H^2 = \mathbb{R} \oplus \mathbb{R}x \oplus H,$$

where $H = \{h \in H^2 : h(0) = 0 \text{ and } h'(0) = 0\}$. Indeed, for all $h \in H^2$, we have $h(x) = h(0) + xh'(0) + g(x)$, where $g(x) := \int_0^x (x-t)h''(t)dt$. Furthermore, the Hilbert space H equipped with the scalar product $(h_1, h_2)_H = \int_0^1 h_1''(t)h_2''(t)dt$ is a RKHS with reproducing kernel $K_x(\cdot) = K(\cdot, x)$ solution of

$$\forall x \in X, h \in H, \quad h(x) = (h, K_x(\cdot))_H = \int_0^1 K_x''(t)h''(t)dt.$$

By a straightforward calculation, one can easily check that

$$K(x, x') = \begin{cases} \frac{x^2}{2}(x' - \frac{x}{3}) & \text{if } x \leq x' \\ \frac{x'}{2}(x - \frac{x'}{3}) & \text{elsewhere.} \end{cases}$$

Using equation (4.5), the optimization problem (4.4) can be expressed as

$$\min_{\substack{h \in H \\ \alpha + \beta x^{(i)} + h(x^{(i)}) = y_i \\ \alpha + \beta x + h(x) \in C}} \int_0^1 (h''(t))^2 dt = \|h\|_H^2.$$

In that case, the discretized optimization problem (P_N) is formulated as

$$(4.6) \quad \arg \min_{\substack{\alpha, \beta, h_N \in H_N \\ \alpha + \beta x^{(i)} + h_N(x^{(i)}) = y_i \\ \alpha + \beta x + h_N(x) \in C}} \|h_N\|_{H_N}^2,$$

Consequently and from Proposition 2.16, the solution of the finite optimization problem (4.6) is equal to

$$\hat{h}_N(x) = \alpha_{opt} + \beta_{opt}x + \sum_{j=1}^N \beta_{opt,j} \varphi_{N,j}(x),$$

where $(\alpha_{opt}, \beta_{opt}, \beta_{opt,1}, \dots, \beta_{opt,N})^\top$ is the solution of the following quadratic optimization problem

$$(4.7) \quad \arg \min_{\substack{\alpha, \beta, \beta_j, j=1, \dots, N \\ \alpha + \beta x^{(i)} + h_N(x^{(i)}) = y_i \\ \alpha + \beta x + h_N(x) \in C}} \gamma^\top \Gamma_N^{-1} \gamma,$$

where $h_N(x) := \sum_{j=1}^N \beta_j \varphi_{N,j}(x)$, $\gamma := (\alpha, \beta, \beta_1, \dots, \beta_N)^\top \in \mathbb{R}^{N+2}$ and $(\Gamma_N)_{i,j} := K(t_{N,i}, t_{N,j})$ $i, j = 1, \dots, N$.

Table 1: Bound observation data on $[0, 1]$.

Variables	Values				
x	0.1	0.15	0.5	0.7	0.95
$f(x)$	-0.1	0.8	-1	0.9	0.1

Table 2: Non-negative observation data on $[0, 1]$.

Variables	Values				
x	0.06	0.12	0.5	0.6	0.95
$f(x)$	0.1	0.8	1	0.4	0.02

4.2. Cubic spline interpolation with bound constraints. In this section, we suppose that the function takes values between -1.2 and 1 (resp. is non-negative on $[0, 1]$) and is evaluated at some points given in Table 1 (resp. Table 2).

The convex set C is the space of functions defined as

$$C = \{f \in \mathcal{C}^0([0, 1]) : -1.2 \leq f(x) \leq 1, x \in [0, 1]\}.$$

In that case, the quadratic optimization problem (4.7) can be formulated as

$$\begin{aligned} \arg \min_{\substack{\alpha, \beta, \beta_j, j=1, \dots, N \\ \alpha + \beta x^{(i)} + h_N(x^{(i)}) = y_i \\ -1.2 \leq \alpha + \beta t_{N,j} + h_N(t_{N,j}) \leq 1}} \gamma^\top \Gamma_N^{-1} \gamma. \end{aligned}$$

The non-negativity constraint can be seen as bound constraints where the lower bound is equal to 0 and the upper bound is equal to $+\infty$. Figure 9 shows the solution \hat{h}_N of the discretized optimization problem (4.6) (red line) and the natural (unconstrained) cubic spline (black line). Only the first one respects both interpolation conditions and bound (resp. non-negativity) constraints in Figure 9a (resp. Figure 9b). Let us mention that the nice result proved by Dontchev in [6] is checked in this numerical example. This result states that the constrained cubic spline is a piecewise third-order polynomial if we add new knots corresponding to saturated constraints (two such knots corresponding to $y = 1$ in Figure 9a).

4.3. Monotone cubic spline interpolation. The aim of this last subsection is to compare the proposed algorithm with existing algorithms for monotone cubic splines interpolation. To do this, we consider a monotone example given in [10] (Fritsch-Carlson (FC), RPN 15A data). These observation data are given in Table 3 and are used to compare different algorithms (for e.g. Akima [1], FC [10] and Hyman [13]).

In Figure 10a, we plot the monotone cubic spline using FC data for four methods: the algorithm described in this paper (red line), Hyman's algorithm (blue line), FC's algorithm (green line) and Akima's algorithm (black line). Only the last one is not monotone everywhere. Figure 10b shows the difference between 'Hyman' and 'FC' splines. To compare these two methods in terms of LE criterion, we plot in Figure 11b the function $f''(x)^2$. Notice that LE criterion for "Hyman" is slightly smaller. So, we compare the proposed algorithm with Hyman's one. Apply equation (4.3) to the analytical expression of the monotone cubic spline calculated in [13], we get

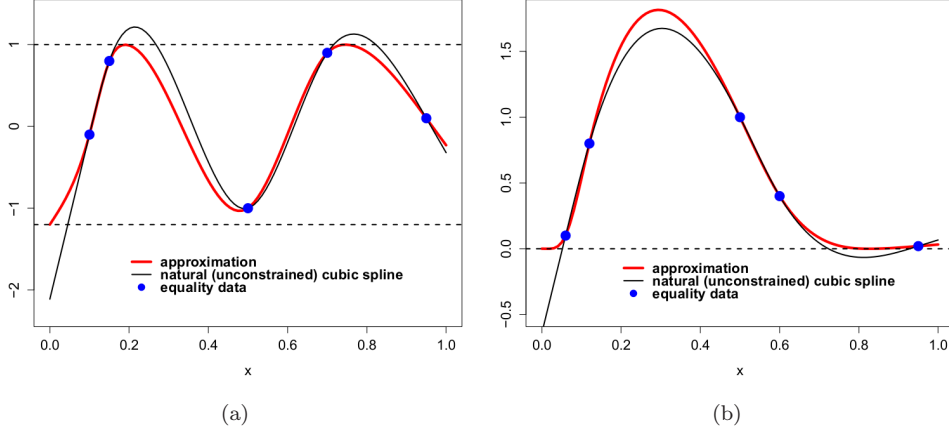


Fig. 9: Bound (resp. non-negative) cubic spline interpolation (red line) using our algorithm in Figure 9a (resp. Figure 9b) and the natural (unconstrained) cubic spline (black line).

Table 3: RPN 15A Fritsch-Carlson's data (LLL radiochemical calculations).

x	$f(x)$
7.99	0
8.09	2.76429e-5
8.19	4.37498e-2
8.7	0.169183
9.2	0.469428
10	0.943740
12	0.998636
15	0.999919
20	0.999994

$E_L = 9.35$. Now, using equation (4.6), the equivalent LE measure of the approximate function \hat{h}_N is defined by

$$\|\hat{h}_N\|_{H_N}^2 = \lambda_N^\top \Gamma_N^{-1} \lambda_N,$$

where $\lambda_N = (\alpha_{opt}, \beta_{opt}, \beta_{opt,1}, \dots, \beta_{opt,N})^\top$. Notice that this approximation converges to the LE criterion of the optimal cubic spline with inequality constraints (see Theorem 2.15). Figure 11a shows the values of $\|\hat{h}\|_{H_N}^2$ for different values of N . One can conclude that these values are much smaller than Hyman's LE measure (for instance $\|\hat{h}\|_{H_N}^2 = 2$ for $N = 100$).

Now, we consider Akima's data [1] which are defined in Table 4. These monotone data are also used in many papers to compare different methods (see e.g. [10], [13] and [25]).

Figure 12 shows the monotone cubic splines for four different methods: the approximation spline described in this paper (red line), Hyman's spline (blue line), FC's

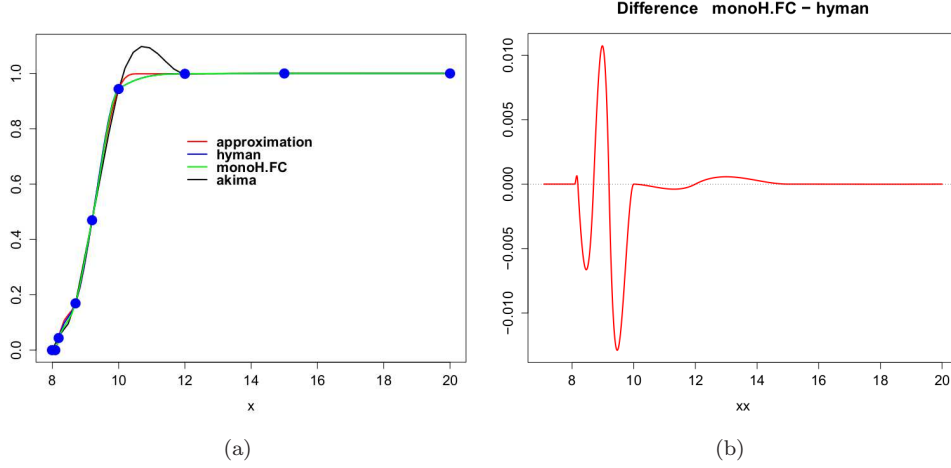


Fig. 10: Monotone cubic spline interpolation for four different methods (Figure 10a). The difference between FC and Hyman splines (Figure 10b).

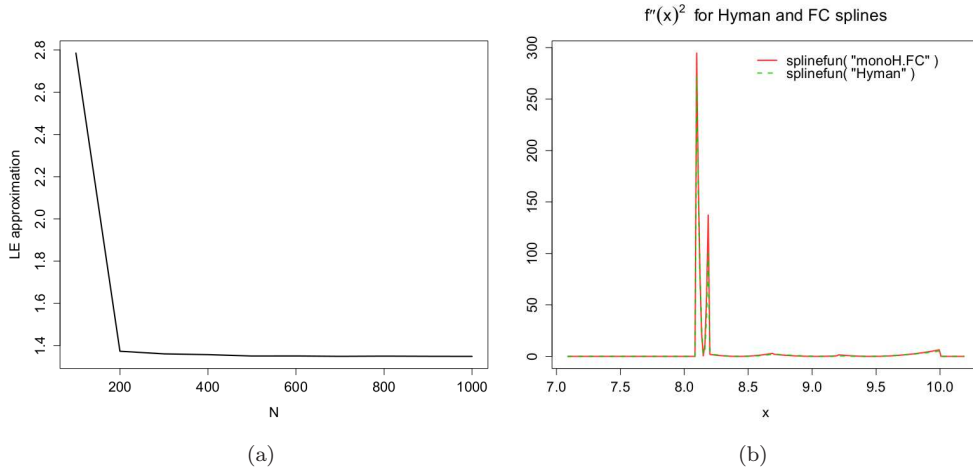


Fig. 11: Approximate LE criterion for the algorithm described in this paper using FC's data (Figure 11a). Comparison between "Hyman" and "FC" splines (Figure 11b).

spline (green line) and Akima's spline (black line). As Fritsch and Carlson [10] wrote in their paper, Akima's method eliminates the "bump" but the interpolant is not monotone on the interval (12, 14). The three other functions are monotone (non-decreasing) everywhere. A comparison between 'Hyman' and 'FC' splines in terms of LE criterion is shown in Figure 13b. Using equation (4.3), the LE criterion for Hyman's method is equal to 8939.78. In Figure 13a, we plot $\|\hat{h}\|_{H_N}^2$ using Akima's data. Notice again that the values are much smaller than Hyman's algorithm.

Table 4: Akima's data used to compare different methods.

Variables	Values										
x	0	2	3	5	6	8	9	11	12	14	15
$f(x)$	10	10	10	10	10	10	10.5	15	50	60	85

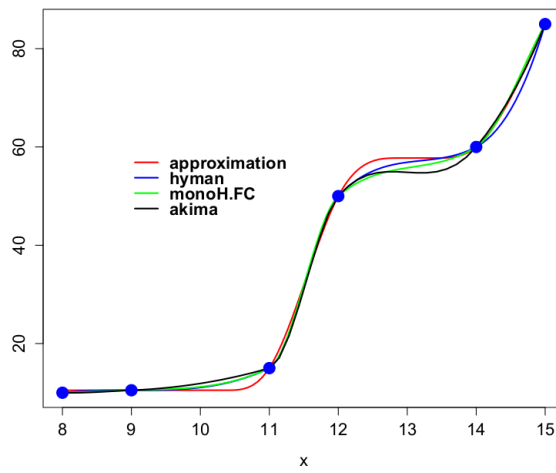


Fig. 12: Monotone cubic splines interpolation for four different methods using Akima's data.

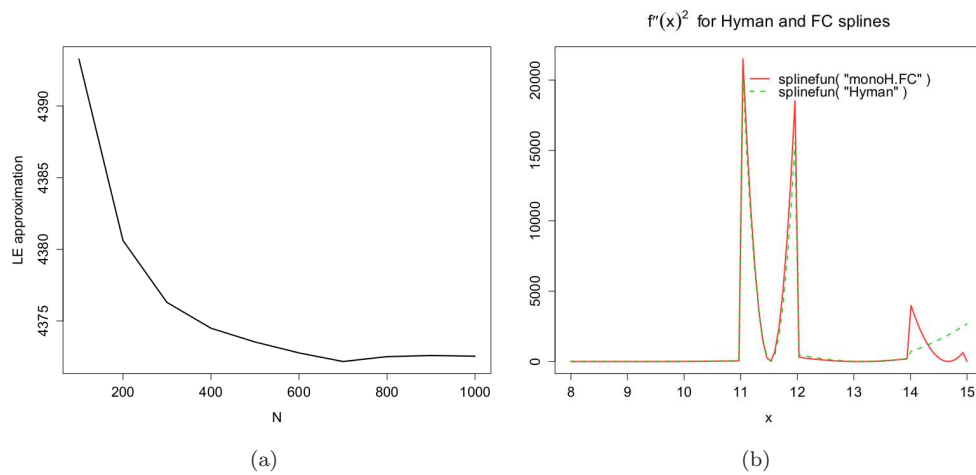


Fig. 13: Approximate LE measure for the algorithm described in this paper using Akima's data. Comparison between "Hyman" and "FC" splines (Figure 11b).

Finally, we consider the monotone Wolberg’s data used in [25] and [26]. These data are given in Table 5 and used to compare our method with seven different algorithms (not described in this paper).

Table 5: Wolberg’s data used to compare different methods.

Variables		Values				
x	0.00	1.00	1.50	2.05	2.90	
$f(x)$	0.00	350.00	354.65	428.00	650.00	

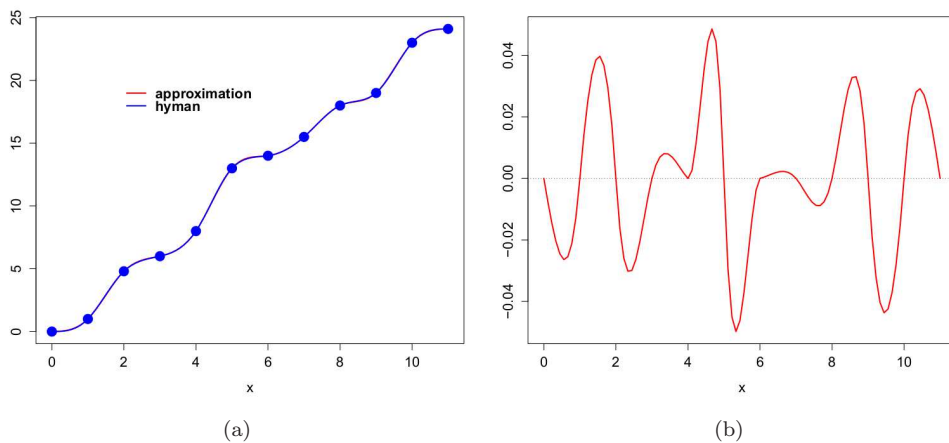


Fig. 14: Monotone cubic splines using Wolberg’s data: Hyman’s method (blue line) and approximation \hat{h}_N with $N = 1000$ (red line). The difference can be seen in Figure 14b.

In Figure 14a, we plot the monotone cubic splines using the method described in this paper (red line) and Hyman’s method (blue line). The difference between these two functions is given in Figure 14b. In Figure 15, we plot $\|\hat{h}\|_{H_N}^2$ and compare with the best LE value in Table 6 (see [25]). Values in Table 6 are taken from Wolberg’s paper ([25]) except for our approximation and Hyman methods.

5. Conclusion. In this work, we consider smoothing and interpolating with inequality constraints as a general convex optimization problem in a Reproducing Kernel Hilbert Space H (RKHS). We assume H continuously embedded in a Banach space E of continuous functions on a compact set X .

A discretized optimization problem in a finite-dimensional Hilbert space H_N is proposed to approximate the optimal constrained interpolating function lying in H . By construction, the corresponding sequence of minimizers in the nested set of spaces H_N satisfy the interpolation conditions and the inequality constraints as functions of the space E .

The main result of this paper is to prove the convergence (with the dimension of

Table 6: Linearized energy measure using Worlberg’s data.

Method	E_L
our approximation	131.68
Hyman	133.19
CSE	132.91
FE	131.68
LE	131.68
SDDE	223.55
MDE	131.71
FB	236.30

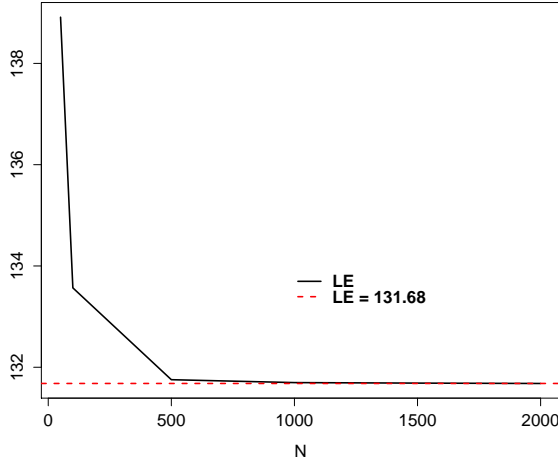


Fig. 15: Approximate LE measure for the algorithm described in this paper using Wolberg’s data.

H_N) of this approximation method in the space E (uniform convergence). Furthermore, the discretized optimization problem is shown to be equivalent to a quadratic program in two standard situations of bound and monotonicity type constraints. Some numerical examples in one and two dimensions are given to show the easy applicability of the method. A first step is to discretize the norm of H (the smoothing criterion) by using explicitly the analytical form of its reproducing kernel. A second important step is to consider approximation spaces H_N such that the (infinite) set of inequality constraints can be reduced to a finite set of inequality constraints in H_N .

Many open problem are left. At first, this paper considers only the simple case of approximation spaces spanned by piecewise linear continuous functions or P1-elements by analogy with the Finite Element Method (for solving PDE). The problem of using other approximation spaces is posed in relation with the regularity of the functions in H (or the reproducing kernel) and the nature of the (inequality) constraints. In the

same way, this paper does not study the order of convergence of the method in relation with the discretization of the domain X (or mesh). At last, a challenging problem is to state the correspondence between this method and a statistical Bayesian approach using the well-known correspondence between splines and Bayesian estimation (see [14]).

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