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Constrained data smoothing via optimal control

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Abstract

The article considers a problem of best smoothing in a strip, where the objective is to find a function $f : [0, 1] \rightarrow \mathbb{R}$ that satisfies bilateral constraints on its values, $d(t) \leq f(t) \leq e(t)$ for all $0 \leq t \leq 1$ and minimizes a weighted sum of the L_2-norm of the second derivative and squared deviations from specified values, y_i, at discrete points $0 = t_1 < t_2 < \cdots < t_{N+2}$. We assume that constraints $d(t)$ and $e(t)$ are continuous functions that are linear in each interval $[t_i, t_{i+1}]$, $i = 1, \ldots, N + 1$. We connect this problem to a state-constrained optimal control problem for the double integrator, and give conditions for the existence and uniqueness of the solution under which we also show that the solution is a cubic spline with knots at t_i and no more than two additional knots in each interval (t_i, t_{i+1}). We propose a numerical algorithm for solving this problem based on a two stage minimization, where the outer loop optimization problem is finite-dimensional and convex, while the inner loop optimization problem admits a solution which is easy to compute. Numerical results that show the efficacy of the proposed approach are reported.

KEYWORDS

data smoothing, optimal control, optimal smoothing, smoothing spline, state constraints

1 | INTRODUCTION

Given data (t_i, y_i) that represent points on the graph of an unknown function, the classical best interpolation problem is to find a function f with minimal L_2 norm of the second derivative whose values at t_i equal y_i. As is well known,[1] the solution of this problem is a natural cubic spline interpolating the data. Dontchev[2] has considered a version of this problem subject to bilateral constraints; namely, the graph of the interpolating function is restricted to a strip defined by two piecewise linear functions across the mesh $\{t_i\}$; it was shown that the solution of this problem is a cubic spline with not more than two additional knots in each interpolation interval (t_i, t_{i+1}). Later[3] the structure of the solution was further characterized as follows. On each interpolation interval one of the four cases may appear: (i) the solution is in the interior of the strip and no additional knots occur; (ii) there is a single point on one of the constraints where the constraint is active (one additional knot); (iii) there is an interval on one of the constraints where this constraint is active (two additional knots on the same constraint); (iv) there are two single points on each of the constraints where the respective constraints are active (two additional knots on different constraints).

In this article we consider a problem of *data smoothing* subject to bilateral constraints representing a strip. By applying optimality conditions and duality in optimal control, we obtain a characterization of the solution which is somewhat similar to that of the best interpolation in a strip,[2,3] but there are important differences. Based on that characterization, we propose an algorithm for data smoothing in a strip and illustrate its effectiveness through computer experiments.

Constrained interpolation and smoothing have been studied from various viewpoints in the past[4-7] and more recently.[8] Specifically, for constrained smoothing, Irvine et al.[9] considered the smoothing problem as an extension of constrained interpolation, where the inequality constraint is imposed on the kth derivative being non-negative, for example, $f^{(k)} \geq 0$. Elfving and Andersson[10] have studied the problem of constrained smoothing splines, where some inequality constraints were imposed on the first derivative f' or second derivative f''. Mammen et al.[11] proposed a unifying framework in a normed vector space for treating constrained smoothing problems; their work also contained an overview of the progress on constrained data smoothing up to the year 2001. Mammen and Thomas-Agnan[12] then employed the framework of Mammen et al.[11] to study the problem of constrained smoothing spline interpolation with monotone shape restriction, that is, $f^{(k)} \geq 0$. Turlach[13] also studied the problem of constrained smoothing spline interpolation with monotone shape restriction and proposed the method which is extendable to multiple simultaneous shape constraints. Kano and Martin[14] studied constrained and optimal smoothing and interpolating splines; the examined constraint types include point, interval, and integrated values. In their work they assumed that the solution function uses the normalized uniform B-splines of some fixed degree k as the basis functions; our work differs by considering f being in a Sobolev space.

It has been known for quite a while that problems in approximation theory have important connections to optimal control,[15] and this connection is also exploited in the present work. In particular, Shen and Wang[16] studied the constrained spline smoothing problem through optimal control; but unlike our work, which deals with the constraints on the state of the reformulated optimal control problem, the work of Shen and Wang deals with the constraint on the control u. Ikeda et al.[17] also addressed the problem of constrained spline smoothing using optimal control; however, the constraints were imposed only at the knots, whereas in this article, we study the case where the bilateral constraints on the function are piecewise linear and imposed pointwise over an interval.

2 PROBLEM SETTING

We consider the following problem:

$$\text{Minimize } \ 0.5\left(\|f''\|_2^2 + \sum_{i,j=1}^{N+2} q_{ij}(f(t_i) - y_i)(f(t_j) - y_j) \right), \tag{1}$$

$$\text{subject to } \ e(t) \leq f(t) \leq d(t) \ \text{ for all } \ t \in [0,1], \ \text{ and } \ f \in W^{2,2}[0,1], \tag{2}$$

where $0 = t_1 < t_2 < \cdots < t_{N+2} = 1$, N is a natural number, y_i, $i \in \{1, 2, \ldots, N+2\}$ are given real numbers, $\|\cdot\|_2$ is the usual L^2 norm of a function on the interval $[0,1]$, and $W^{2,2}[0,1]$ denotes the Sobolev space of functions on $[0,1]$ with absolutely continuous first derivatives and second derivative in L^2. In the problem described by (1) and (2), the first term is the standard in best interpolation problems squared L^2 norm of the second derivative of f, while the second term represents least squares with weights q_{ij} of the deviation of values of f at t_j from given points y_j. The functions d and e describe a strip where the values of the function f should belong.

We denote by $Q \in \mathbb{R}^{(N+2)\times(N+2)}$ the square matrix $[q_{ij}]$ and we assume that Q is symmetric and positive semi-definite $Q = Q^{\mathrm{T}} \succcurlyeq 0$. Furthermore, there exist i, j, $i < j$, such that

$$\tilde{Q} = \begin{bmatrix} q_{ii} & q_{ij} \\ q_{ji} & q_{jj} \end{bmatrix} \succ 0. \tag{3}$$

Condition (3) could be satisfied, for instance, by choosing weights q_{ii} and q_{jj} at some two points t_i and t_j to be positive while selecting the corresponding cross-weights q_{ij} and q_{ji} to be zero.

We assume that the functions e and d are piecewise linear and continuous across the knots t_i and such that $e(t) < d(t)$ for all $t \in [0,1]$. Furthermore, we assume that

$$e(t_j) < y_j < d(t_j), \quad j = 1, \ldots, N+2. \tag{4}$$

Indeed, we need to find a best fit of the points y_i with a function having values in the strip, hence it should be expected that the points (t_i, y_i) are inside the strip. Without the strip constraint, the solution to this problem is the well-known smoothing cubic spline.[1]

We will now prove the existence and uniqueness of solution by reformulating the problem as an optimal control problem. Let $x_1 = f, x_2 = f', u = f''$. Then problem (1) and (2) can be written in the following form:

$$\text{Minimize } J = 0.5\left(\|u\|_2^2 + \sum_{i,j=1}^{N+2} q_{ij}(x_1(t_i) - y_i)(x_1(t_j) - y_j)\right), \tag{5}$$

$$\begin{aligned} \text{subject to } \; & \dot{x}_1 = x_2, \\ & \dot{x}_2 = u, \end{aligned}$$

$$\text{and } \; u \in \mathcal{U} = \{u \in L^2[0,1] | \exists x_1 \text{ with } \ddot{x}_1(t) = u(t) \text{ a.e. } 0 \le t \le 1 \text{ and } e(t) \le x_1(t) \le d(t) \text{ for all } t \in [0,1]\}. \tag{6}$$

Note that in the optimal control problem we interpret t as time and we use dots to designate time derivatives. This is a (nonstandard) optimal control problem for the double integrator, where u is the control and $x = (x_1, x_2)$ is the state. Note that the inequality state constraints appear in the definition of the feasible set $\mathcal{U}$ for the control.

The set $\mathcal{U}$ is clearly convex. It is also closed. Indeed, suppose $u^n \in \mathcal{U}$, $u^n \to \bar{u}$ in L_2 and let x_1^n be the corresponding x_1. Note that

$$x_1^n(t) = x_1^n(0) + t\left(x_1^n(1) - x_1^n(0) - \int_0^1 (t-\sigma)u^n(\sigma)d\sigma\right) + \int_0^t (t-\sigma)u^n(\sigma)d\sigma. \tag{7}$$

The sequences of real numbers $x_1^n(0)$ and $x_1^n(1)$ are bounded between $e(0)$ and $d(0)$ and between $e(1)$ and $d(1)$, respectively; hence we can extract their convergent subsequences to some $\bar{x}_1(0)$ and $\bar{x}_1(1)$, respectively. Without loss of generality, we can assume that the original sequences $x_1^n(0)$ and $x_1^n(1)$ converge to $\bar{x}_1(0)$ and $\bar{x}_1(1)$ while $u^n \to \bar{u}$ in L_2 as $n \to \infty$. Define $\bar{x}_1$ by boundary conditions $\bar{x}_1(0)$ and $\bar{x}_1(1)$ and $\ddot{\bar{x}}_1 = \bar{u}$, that is,

$$\bar{x}_1(t) = \bar{x}_1(0) + t\left(\bar{x}_1(1) - \bar{x}_1(0) - \int_0^1 (t-\sigma)\bar{u}(\sigma)d\sigma\right) + \int_0^t (t-\sigma)\bar{u}(\sigma)d\sigma. \tag{8}$$

Exploiting Cauchy–Schwartz inequality in the expression for $|x_1^n(t) - \bar{x}_1(t)|$ formed using (7) and (8), we obtain that L^2 convergence of controls and convergence of boundary conditions implies uniform (C^0) convergence of the corresponding state trajectories, that is, $x_1^n \to \bar{x}_1$ as $n \to \infty$. Thus $e(t) \le \bar{x}_1(t) \le d(t)$ for all $0 \le t \le 1$ and $\bar{u} \in \mathcal{U}$.

Based on condition (4), we will now show that there exists a feasible trajectory of the state x_1 whose values at t_j are in the interior of the strip. Let f_0 be the piecewise linear function whose graph connects the points (t_i, y_i). Clearly, $e(t) < f_0(t) < d(t)$ for all $t \in [0,1]$. For any natural m, let $t_{i,j} = t_i + j(t_{i+1} - t_i)/m$. It is well known that there exists a sequence S_m of cubic splines interpolating points $(t_{i,j}, f_0(t_{ij}))$ that converges to f_0 uniformly in $[0,1]$. Then for m sufficiently large we will have $e(t) < S_m(t) < d(t)$ for all $t \in [0,1]$. Thus, S_m is a feasible trajectory for the state x_1 with values in the interior of the strip, and the second time-derivative of S_m is a feasible control for which the value of the objective function is finite. This yields that there exists a sublevel set of J in (5), viewed as a function of u, which is nonempty; it is obviously closed and convex in L^2. Since

$$0.5\|u\|_2^2 \le J(u) \text{ for all } u \in L^2,$$

the sublevel sets are furthermore bounded, hence weakly compact.

The rest of the proof of the existence is standard. The intersections of the nonempty sublevel set with the feasible set $\mathcal{U}$ is weakly compact too and the minimization over this intersection is equivalent to the minimization over $\mathcal{U}$. The objective function is convex and continuous, hence weakly lower semicontinuous. Thus, under the assumption made, problem (5) and (6) has a solution and hence problem (1) and (2) has a solution.

The condition (3) ensures that J in (5), viewed as a function of x_1, is strictly convex*. This gives us uniqueness of the solution.

We denote the solution by $(\bar{x}, \bar{u}, \bar{z})$. In the following section we will show that the solution $\bar{x}_1$ is in fact a cubic spline with no more than 2 additional knots in each interval $[t_i, t_{i+1}]$. We also give a detailed description of the solution together with an algorithm to compute it.

3 CHARACTERIZING THE SOLUTION

Suppose $f \in W^{2,2}[0,1]$ and $0 = t_1 < t_2 < \cdots t_{N+2} = 1$ are given. The ith normalized linear B-spline is defined by:[1]

$$B_i(t) = \begin{cases} 0 & \text{if } t_{i+2} < t, \\ \frac{t_{i+2}-t}{t_{i+2}-t_{i+1}} & \text{if } t_{i+1} < t \le t_{i+2}, \\ \frac{t_{i+2}-t}{t_{i+2}-t_{i+1}} - \frac{t_{i+1}-t}{t_{i+2}-t_{i+1}} - \frac{t_{i+1}-t}{t_{i+1}-t_i} & \text{if } t_i < t \le t_{i+1}, \\ 0 & \text{if } t \le t_i. \end{cases}$$

Integrating by parts, it follows that

$$\begin{aligned} \int_0^1 f''(t)B_i(t)dt &= \int_{t_i}^{t_{i+1}} f''(t)B_i(t)dt + \int_{t_{i+1}}^{t_{i+2}} f''(t)B_i(t)dt \\ &= \left(-f'(t_{i+1}) + \frac{f(t_{i+2}) - f(t_{i+1})}{t_{i+2} - t_{i+1}}\right) + \left(f'(t_{i+1}) - \frac{f(t_{i+1}) - f(t_i)}{t_{i+1} - t_i}\right) \\ &= \frac{f(t_{i+2}) - f(t_{i+1})}{t_{i+2} - t_{i+1}} - \frac{f(t_{i+1}) - f(t_i)}{t_{i+1} - t_i}. \end{aligned}$$

Defining the vector function $B(t) = (B_i)_{i=1}^N = (B_1(t), \ldots, B_N(t))^T$, where B_i's are as above, we have

$$\int_0^1 f''(t)B(t)dt = \begin{pmatrix} \frac{f(t_3)-f(t_2)}{t_3-t_2} - \frac{f(t_2)-f(t_1)}{t_2-t_1} \\ \frac{f(t_4)-f(t_3)}{t_4-t_3} - \frac{f(t_3)-f(t_2)}{t_3-t_2} \\ \vdots \\ \frac{f(t_{N+2})-f(t_{N+1})}{t_{N+2}-t_{N+1}} - \frac{f(t_{N+1})-f(t_N)}{t_{N+1}-t_N} \end{pmatrix} = Kz,$$

where

$$K = \begin{bmatrix} \frac{1}{t_2-t_1} & -\frac{t_3-t_1}{(t_3-t_2)(t_2-t_1)} & \frac{1}{t_3-t_2} & 0 & \cdots & 0 & 0 & 0 \\ 0 & \frac{1}{t_3-t_2} & -\frac{t_4-t_2}{(t_4-t_3)(t_3-t_2)} & \frac{1}{t_2-t_1} & \cdots & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \cdots & \ddots & \ddots & 0 \\ 0 & 0 & 0 & 0 & \cdots & \frac{1}{t_{N+1}-t_N} & -\frac{t_{N+2}-t_N}{(t_{N+2}-t_{N+1})(t_{N+1}-t_N)} & \frac{1}{t_{N+2}-t_{N+1}} \end{bmatrix},$$

$$z = \begin{pmatrix} f(t_1) \\ f(t_2) \\ f(t_3) \\ \vdots \\ f(t_N) \\ f(t_{N+1}) \\ f(t_{N+2}) \end{pmatrix}.$$

Because $t_1 < t_2 < \cdots < t_{N+2}$, the rows of K must be linearly independent, that is, $K \in \mathbb{R}^{N\times(N+2)}$ is full row rank.

Let $y = (y_1, y_2, \dots, y_{N+2})^{\mathrm{T}}$. As in Section 2, denoting $x_1 = f, x_2 = f', u = f''$, problem (1) and (2) can be written in the following form:

$$\begin{aligned}
&\text{Minimize with respect to } (x, u, z) \in W^{2,2} \times L^2 \times \mathbb{R}^{N+2} \\
&\text{the objective function } J(x, z, u) = \frac{1}{2}\left(\|u\|_2^2 + (z-y)^{\mathrm{T}} Q (z-y)\right) \\
&\text{subject to } \dot{x}_1 = x_2, \quad x_1(t_i) = z_i, \text{ for } i \in \{1, \dots, N+2\} \\
&\qquad \dot{x}_2 = u, \\
&\qquad e(t) \le x_1(t) \le d(t) \text{ for all } t \in [0,1], \\
&\qquad \int_0^1 u(t)B(t)dt = Kz.
\end{aligned} \tag{9}$$

In this section we employ the duality theory and optimality conditions for state and control constrained optimal control problems developed by Hagger and Mitter[18] and previously applied by Dontchev[2] to the best interpolation in a strip problem. First, observe that, as shown in the preceding section, condition (4) implies that there exists a feasible control u such that the corresponding trajectory of the state x_1 satisfies $e(t) < x_1(t) < d(t)$ for all $t \in [0,1]$. This, combined with the surjectivity of the matrix K, implies that Slater's constraint qualification holds, hence we can apply the Lagrange multiplier rule.

To do that, we introduce the Lagrange functional

$$\begin{aligned}
\mathcal{L}(x, x(0), z, u, \lambda, \nu, \mu) = J(x, z, u) + \lambda^T \left(\int_0^1 u(t)B(t)dt - Kz\right) + \int_0^1 \left[x_1(t) - x_1(0) - \int_0^t x_2(s)ds\right] d\nu_1 \\
+ \int_0^1 \left[x_2(t) - x_2(0) - \int_0^t u(s)ds\right] d\nu_2 + \int_0^1 (e - x_1)d\mu_1 + \int_0^1 (x_1 - d)d\mu_2,
\end{aligned}$$

where $\lambda = (\lambda_1, \dots, \lambda_N)^{\mathrm{T}} \in \mathbb{R}^N$, $\nu = (\nu_1, \nu_2)$ is a regular Borel measure, and $\mu = (\mu_1, \mu_2)$ is a nonnegative regular Borel measure such that μ_1 is supported on the set $T_1 = \{t \in [0,1], x_1(t) = e(t)\}$ and μ_2 is supported on the set $T_2 = \{t \in [0,1], x_1(t) = d(t)\}$. Based on separation of convex sets by a hyperplane, one can show, following similar arguments as by Dontchev,[2] that there exist optimal Lagrange multipliers $(\overline{\lambda}, \overline{\nu}, \overline{\mu})$ such that

$$\mathcal{L}(\overline{x}, \overline{x}(0), \overline{z}, \bar{u}, \overline{\lambda}, \overline{\nu}, \overline{\mu}) \le \mathcal{L}(x, \alpha, z, u, \overline{\lambda}, \overline{\nu}, \overline{\mu}), \tag{10}$$

for every continuous function x with $x(t) \in \mathbb{R}^2, t \in [0,1]$, every $\alpha \in \mathbb{R}^2$, every $z \in \mathbb{R}^{N+2}$, and every $u \in L^2$.

Define

$$\overline{p}_1(t) = \int_t^1 d\overline{\nu}_1, \quad \overline{p}_2(t) = \int_t^1 d\overline{\nu}_2. \tag{11}$$

Then $\overline{p}_1$ and $\overline{p}_2$ are functions of bounded variations that are continuous from the left. Since the Lagrange functional is convex and Fréchet differentiable, the condition (10) is equivalent to the corresponding optimality condition based on the Fermat rule "derivative equals zero." Differentiating $\mathcal{L}$ with respect to z and evaluating at the optimal variables results in

$$Q(\overline{z} - y) + K^T \overline{\lambda} = 0. \tag{12}$$

Next, differentiating $\mathcal{L}$ with respect to $x(0) = (x_1(0), x_2(0))$ and evaluating at the optimal variables gives

$$\overline{p}_1(0) = \overline{p}_2(0) = 0.$$

Since

$$\int_0^t \int_1^t \bar{u}(s)dsd\overline{\nu}_2 = \int_0^1 \bar{u}(t)\overline{p}_2(t)dt,$$

from the equality $\partial\mathcal{L}/\partial u = 0$ evaluated at the optimal variables we get

$$\bar{u}(t) + B(t)^T\overline{\lambda} - \overline{p}_2(t) = 0. \tag{13}$$

Furthermore, utilizing the equality

$$\int_0^1 \overline{x}_2 d\overline{v}_2 - \int_0^1\int_0^t dsd\overline{v}_2 = \int_0^1 \overline{x}_2 d(-\overline{p}_2 + \int_s^1 \overline{p}_1),$$

and differentiating $\mathcal{L}$ with respect to x_2 gives

$$\dot{\overline{p}}_2 = -\overline{p}_1, \quad \overline{p}_2(0) = 0. \tag{14}$$

Note that $\overline{p}_1$ and $\overline{p}_2$ are the familiar from Pontryagin's maximum principle adjoint variables. Finally, differentiating $\mathcal{L}$ with respect to x_1 results in

$$\overline{p}_1(t) = -\int_t^1 d(\overline{\mu}_2 - \overline{\mu}_1). \tag{15}$$

We conclude from (13) that the optimal control $\bar{u}$ is an absolutely continuous function which is the sum of a piecewise linear and continuous function across the knots t_i and an absolutely continuous function whose derivative, as given in (14), is of the form (15) with $\overline{\mu}_i$, $i = 1, 2$, being nonnegative regular measures supported on the disjoint subsets T_i of $[0, 1]$ where the state constraints are active. In addition, (13), $\overline{p}_2(0) = 0$, (11) (implying $\overline{p}_2(1) = 0$), and $B(0) = B(1) = 0$ give that the optimal control satisfies $\bar{u}(0) = \bar{u}(1) = 0$.

Let τ_1, τ_2 be such that for the optimal solution $\overline{x}_1$ satisfies $e(t) < \overline{x}_1(t) < d(t)$ for all $t \in (\tau_1, \tau_2)$. From (15) we have that $\overline{p}_1(t) = 0$, hence from (14) the adjoint variable $\overline{p}_2$ is constant. Thus, from (13), on such an interval (τ_1, τ_2) the optimal control $\bar{u}(t)$ is a piecewise linear continuous function. Furthermore, in the case when the interval (τ_1, τ_2) is contained in some of the intervals (t_j, t_{j+1}), the optimal $\bar{u}$ is a linear function inasmuch B_j is linear there. Then the optimal $\overline{x}_2$ is a quadratic polynomial there while the optimal $\overline{x}_1$ is a cubic polynomial.

Assume that in some interval (t_j, t_{j+1}) there are two points τ_1 and τ_2, $t_i \le \tau_1 < \tau_2 \le t_{i+1}$ such that $\overline{x}_1(\tau_1) = e(\tau_1)$ and $\overline{x}_1(\tau_2) = e(\tau_2)$. Let $\zeta(t) = 0$ for $t \in (\tau_1, \tau_2)$ and $\zeta(t) = \bar{u}(t)$ for $t \notin (\tau_1, \tau_2)$. Note that $\overline{x}_1(\tau_2) = e(\tau_2)$ and $\overline{x}_2(\tau_2) = \dot{e}(\tau_2)$ since $\overline{x}_2 - e$ is maximized at τ_2. Apply the control ζ to the double integrator with the optimal initial conditions $\overline{x}_1(0)$ and $\overline{x}_2(0)$ obtaining trajectories $\xi = (\xi_1, \xi_2)$. Clearly, $\xi_i(t) = \overline{x}_i(t)$ for $t \in [0, \tau_1]$. Since $\zeta(t) = 0$ on $[\tau_1, \tau_2]$, we have that $\xi_1(t) = e(t)$ on $[\tau_1, \tau_2)$. Then we also have $\xi_1(\tau_2) = e(\tau_2) = \overline{x}_1(\tau_2)$ and $\xi_2(\tau_2) = \dot{e}(\tau_2) = \overline{x}_2(\tau_2)$. But then $\xi_i(t) = \overline{x}_i(t)$ for $t \in [\tau_2, 1]$, $i \in \{1, 2\}$. Thus, we found a function $\xi_1(t)$ such that $\xi_1(t_i) = \overline{x}_1(t_i)$ and also $\ddot{\xi}_1(t) = 0$ on $[\tau_1, \tau_2]$. If we assume that $\bar{u}(v) = \ddot{\overline{x}}_1(v) \neq 0$ for some $v \in ([\tau_1, \tau_2)$, since $\bar{u}$ is a continuous function, there exists $\varepsilon > 0$ such that $\bar{u}(t) = \ddot{\overline{x}}_1(t) \neq 0$ in $(v - \varepsilon, v + \varepsilon)$ and then the value of the objective function of (9) will be greater than the value obtained for the function $\zeta(t) = \ddot{\xi}_1(t)$ and ξ_1. This contradicts the optimality of $\bar{u}$. We conclude that when $\overline{x}_1(\tau_1) = e(\tau_1)$ and $\overline{x}_1(\tau_2) = e(\tau_2)$ for $t_j \le \tau_1 < \tau_2 \le t_{j+1}$ then $\overline{x}_1(t) = e(t)$ for all $t \in [\tau_1, \tau_2]$; moreover, $\bar{u}(t) = 0$ for all $t \in [\tau_1, \tau_2]$ as well. Clearly, the same argument works for the lower constraint d.

The property of the solution $\overline{x}_1$ we found means that each of the constraints cannot be active in two separate (isolated) points in (t_i, t_{i+1}). That is, in every (t_i, t_{i+1}) each of the constraints is active either at one point, or on an interval. We will also show that if one of the constraints is active on an interval with positive length in $[t_i, t_{i+1}]$ the other constraint cannot be active in (t_i, t_{i+1}). We summarize and complement our findings in the following theorem:

Theorem 1. *If one of the constraints is active on an interval with positive length in* $[t_i, t_{i+1}]$ *the other constraint cannot be active in* (t_i, t_{i+1})*. This implies that the solution* $\overline{x}_1$ *is a cubic spline with knots at* t_i*,* $i = 1, \ldots, N + 2$*, and at most two additional knots in each* (t_i, t_{i+1})*,* $i = 1, \ldots, N + 1$*.*

Proof. Suppose that both constraints are active somewhere in $[t_i, t_{i+1}]$ and such that one of the constraints is active on an interval with positive length. Let τ_1, τ_2 be two additional consecutive knots in (t_i, t_{i+1}) that belong to two different constraints; assume also $\tau_1 < \tau_2$. There are four cases to be considered:

1. τ_1 is the right end of a proper interval where the lower constraint e is active.

2. τ_1 is the right end of a proper interval where the upper constraint d is active.
3. τ_1 is a single (isolated) point where lower constraint e is active, meaning that τ_2 is the left end of a proper interval where the upper constraint d is active.
4. τ_1 is a single (isolated) point where the upper constraint d is active, meaning that τ_2 is the left end of a proper interval where the lower constraint e is active.

Consider the first case and let $\overline{x}_1$ be the solution. Note that $e(t) < \overline{x}_1(t) < d(t)$ for $t \in (\tau_1, \tau_2)$. Since $\ddot{\overline{x}}_1(t) = \ddot{e}(t) = 0$ for $t < \tau_1$ and close to τ_1, and since $\ddot{\overline{x}}_1$ is continuous on $(0, 1)$, it follows that $\ddot{\overline{x}}_1(\tau_1) = 0$.

From (13), (12) and the fact that K is full rank, we have that

$$\overline{\lambda} = -(KK^{\mathrm{T}})^{-1}KQ(\overline{z} - y),$$

and for $t \in (\tau_1, \tau_2)$,

$$\dddot{\overline{x}}_1(t) = \dot{B}(t)^{\mathrm{T}}(KK^{\mathrm{T}})^{-1}KQ(\overline{z} - y) + \int_t^1 d(\overline{\mu}_1 - \overline{\mu}_2). \tag{16}$$

Since $\dot{B}(t)$ is a constant for $t \in (t_i, t_{i+1})$, $\overline{\mu}_2(t) = 0$ and $\overline{\mu}_1(t) \geq 0$ for $t \in (t_i, \tau_1)$ and $\overline{\mu}_1(t) = 0$ for $t \in (\tau_1, \tau_2)$, it follows that $\dddot{\overline{x}}_1(t) \geq 0$ for $t \in (\tau_1, \tau_2)$. Note that $\dddot{\overline{x}}_1$ is also a constant on (τ_1, τ_2). Thus $\ddot{\overline{x}}_1(t)$ is non-decreasing for $t \in (\tau_1, \tau_2)$, $\ddot{\overline{x}}_1(\tau_1) = 0$, and hence $\ddot{\overline{x}}_1(t) \geq 0$ for all $t < \tau_2$ that are close to τ_2. On the other hand, since $\ddot{\overline{x}}_1$ is continuous in $(0, 1)$, by the Taylor theorem, for every $t \in (\tau_1, \tau_2)$, we have

$$\begin{aligned}
\overline{x}_1(t) &= \overline{x}_1(\tau_2) + \dot{\overline{x}}_1(\tau_2)(t - \tau_2) + \frac{1}{2}\ddot{\overline{x}}_1(\overline{\tau})(t - \tau_2)^2 \\
&= d(t) + \frac{1}{2}\ddot{\overline{x}}_1(\overline{\tau})(t - \tau_2)^2,
\end{aligned}$$

for some $\overline{\tau} \in [t, \tau_2]$. This follows since $\overline{x}_1(\tau_2) = d(\tau_2)$, and $\dot{\overline{x}}_1(\tau_2) = \dot{d}(\tau_2)$ as $\overline{x}_1 - d$ has a maximum at $t = \tau_2$, while $d(t) = d(\tau_2) + \dot{d}(\tau_2)(t - \tau_2)$ for $t \in [\tau_1, \tau_2]$ since $d(t)$ is linear. Since $\overline{x}_1(t) < d(t)$ for $t \in (\tau_1, \tau_2$, there exist time instants $t < \tau_2$ arbitrary close to τ_2 where $\ddot{\overline{x}}_1(t) < 0$. Consequently, Case 1 cannot occur.

The rest of the cases is analyzed similarly. Therefore, the solution can only have at most two additional knots in $[t_i, t_{i+1}]$. ■

4 | REDUCTION TO TWO STAGE MINIMIZATION

Given any $f \in W^{2,2}[0, 1]$, let $\eta(f)$ be a vector with components $f(t_i)$ and $\theta(f)$ be a vector with components $f'(t_i)$, $i = 1, 2, \dots, N + 2$. Let

$$J(f) = 0.5\left(\|f''\|_2^2 + (\eta(f) - y)^{\mathrm{T}}Q(\eta(f) - y)\right),$$

and consider the problem (1) and (2) which can be restated as

$$\text{Minimize } J(f) \text{ subject to } f \in W^{2,2}[0, 1],\ e(t) \leq f(t) \leq d(t). \tag{17}$$

Define $\varphi(\eta, \theta)$ as the value function of the following optimization problem:

$$\begin{aligned}
\text{Minimize } & 0.5\left(\|f''\|_2^2 + (\eta - y)^{\mathrm{T}}Q(\eta - y)\right) \\
\text{subject to } & f(t_i) = \eta_i,\ f'(t_i) = \theta_i,\ i = 1, \dots, N + 2, \\
& e(t) \leq f(t) \leq d(t),\ 0 \leq t \leq 1, \\
& f \in W^{2,2}[0, 1].
\end{aligned} \tag{18}$$

We let $\varphi(\eta, \theta) = +\infty$ if a feasible solution to (18) does not exist. Consider the problem:

$$\begin{aligned} &\text{Minimize } \ \varphi(\eta, \theta) \\ &\text{subject to } \ \eta \in \mathcal{E} := \{\eta \in \mathbb{R}^{N+2} : \ e(t_i) \le \eta_i \le d(t_i), \ i = 1, \dots, N+2\} \ \text{ and } \theta \in \mathbb{R}^{N+2}. \end{aligned} \tag{19}$$

The solution to (19) exists and is unique. Indeed, let f^* be the unique solution to (1) and (2), and define $\eta^* = \eta(f^*)$, $\theta^* = \theta(f^*)$. If there exists f^{**} which is feasible for (18) for some η^{**}, θ^{**} and $\varphi(\eta^{**}, \theta^{**}) \le \varphi(\eta^*, \theta^*)$ then

$$J(f^{**}) = \varphi(\eta^{**}, \theta^{**}) \le \varphi(\eta^*, \theta^*) = J(f^*).$$

Since f^{**} is feasible for (1) and (2), this is only possible if $f^{**} = f^*$ and $\eta^{**} = \eta^*$, $\theta^{**} = \theta^*$. By an analogous argument, solving problem (18) and (19) should lead to the same solution as solving the original problem (1) and (2).

The problem (19) is a convex finite-dimensional optimization problem. Furthermore, the solution to problem (18) can be easily computed.

For completeness, we demonstrate that the function φ is strictly convex. Let $\eta^1, \ \eta^2 \in [e(t_1), d(t_1)] \times \cdots \times [e(t_{N+2}), d(t_{N+2})]$ and $\theta^1, \ \theta^2 \in \mathbb{R}^{N+2}$. Let f^1 and f^2 be the solutions to (18) which correspond to η^1, θ^1 and η^2, θ^2, respectively. Consider $\lambda \in (0, 1)$ and $\eta^0 = \lambda\eta^1 + (1-\lambda)\eta^2$, $\theta^0 = \lambda\theta^1 + (1-\lambda)\theta^2$, $f^\lambda = \lambda f^1 + (1-\lambda)f^2$. Then f^λ is feasible for (18) with $\eta = \eta^0, \theta = \theta^0$. Let f^0 denote the solution to (18) corresponding to η^0, θ^0. Note that $2\varphi(\eta, \theta)$ can be decomposed into a sum of a function: A function

$$2\tilde{\varphi}(\eta, \theta) = \|(f)''\|_2^2 + (\tilde{\eta} - \tilde{y})^{\mathrm{T}} \tilde{Q} (\tilde{\eta} - \tilde{y}), \tag{20}$$

and another convex function, where $\tilde{\eta}, \tilde{y}$ are 2×1 vectors consisting of ith and jth components of η and y, respectively, and i, j, and $\tilde{Q}$ are identified in (3). Hence it is sufficient to show strict convexity of $2\tilde{\varphi}(\eta, \theta)$. From $\tilde{Q} \succ 0$, optimality of f^0 for η^0, θ^0 and strict convexity of the L_2 norm squared, we have

$$\begin{aligned} 2\tilde{\varphi}(\eta^0, \theta^0) &= \|(f^0)''\|_2^2 + (\tilde{\eta}^0 - y)^{\mathrm{T}} \tilde{Q} (\tilde{\eta}^0 - \tilde{y}) \\ &\le \|(f^\lambda)''\|_2^2 \\ &\quad + (\lambda(\tilde{\eta}^1 - y) + (1-\lambda)(\tilde{\eta}^2 - \tilde{y}))^{\mathrm{T}} \tilde{Q} (\lambda(\tilde{\eta}^1 - \tilde{y}) + (1-\lambda)(\tilde{\eta}^2 - \tilde{y})) \\ &\le \lambda \|(f^1)''\|_2^2 + (1-\lambda)\|(f^2)''\|_2^2 \\ &\quad + \lambda(\tilde{\eta}^1 - \tilde{y})^{\mathrm{T}} \tilde{Q} (\tilde{\eta}^1 - \tilde{y}) + (1-\lambda)(\tilde{\eta}^2 - \tilde{y})^{\mathrm{T}} \tilde{Q} (\tilde{\eta}^2 - \tilde{y}), \end{aligned}$$

where the equality is only possible if $(f^1)''(t) = (f^2)''(t)$ for almost all $0 \le t \le 1$ and $\tilde{\eta}^1 = \tilde{\eta}^2$, that is, $f^1(t_i) = f^2(t_i), f^1(t_j) = f^2(t_j)$. But this implies $f^1 = f^2$ and hence $\eta^1 = \eta^2$ and $\theta^1 = \theta^2$. This proves strict convexity.

Given a set of values $\{\eta_i\}_{i=1}^{N+2}$, $\{\theta_i\}_{i=1}^{N+2}$, $\eta = (\eta_1, \dots, \eta_{N+2})^{\mathrm{T}}$ and $Q \succcurlyeq 0$, $\varphi(\eta, \theta)$ can be computed as

$$\varphi(\eta, \theta) = 0.5 \left[\sum_{i=1}^{N+1} \varphi_i(\eta_i, \theta_i, \eta_{i+1}, \theta_{i+1}) \right] + 0.5(\eta - y)^{\mathrm{T}} Q (\eta - y),$$

where φ_i is the value function of the following optimization problem for the interval $[t_i, t_{i+1}]$:

$$\text{Minimize } \ \|f''\|^2_{L^2[t_i, t_{i+1}]}, \tag{21}$$

$$\text{subject to } \ f(t_i) = \eta_i, \ f'(t_i) = \theta_i, f(t_{i+1}) = \eta_{i+1}, \ f'(t_{i+1}) = \theta_{i+1}, \tag{22}$$

$$e(t) \le f(t) \le d(t) \ \text{ for } \ t_i \le t \le t_{i+1}, \ \text{ and } \ f \in W^{2,2}[t_i, t_{i+1}].$$

Thus the inner-loop optimization problem (18) can be broken down into $N + 1$ independent problems. Note that each of these optimization problems is convex in $W^{2,2}[t_i, t_{i+1}]$ but infinite-dimensional. By the same arguments as in the proof of Theorem 1 (see also a similar treatment in Reference 7), the solution to (21) and (22) is a cubic spline for which one of the following holds in each interval (t_i, t_{i+1}):

1. The constraints are not active (Case 0).
2. A constraint is active at a single (isolated) point either on the lower constraint e (Case 1) or on the upper constraint d (Case 2). The point where the constraint is active is called a *touching point*.
3. A constraint is active on a proper interval; the segment on the constraint that is active is refereed to as the *subarc*. The subarc can be on a lower constraint (Case 3) or on the upper constraint (Case 4).
4. The solution touches lower constraint at a single (isolated) point first and then the upper constraint at a single (isolated) point (Case 5) or the upper constraint first at a single (isolated) point and then the lower constraint at a single (isolated) point (Case 6). Such a solution is said to have a *touching pair* in $[t_i, t_{i+1}]$

As it will become clear from Section 5, the numerical complexity of solving (21) and (22) primarily stems from Cases 5 and 6 that need to be handled numerically (Cases 0–4 can be solved analytically), and from the objective function of (19) being differentiable almost everywhere yet potentially not everywhere. Strategies for addressing Cases 5 and 6 are further discussed in Section 5 while a plethora of algorithms for nondifferentiable optimization[19] is available for nonsmooth problems.

5 | NUMERICAL IMPLEMENTATION AND EXAMPLES

The numerical implementation has been carried out in MATLAB 2021a using the Optimization Toolbox and the Curve Fitting Toolbox. The codebase written for this article is uploaded to GitLab; its URL is included at the end of this article.

The process of numerically solving the problem involves a two stage optimization. In the inner loop, independent problems (21) and (22) are solved by constructing solution candidates for each of 7 cases (if exist) and selecting the one that has the smallest L_2-norm. In the outer loop, the function φ is minimized in its domain. To reliably distinguish between the touching point and subarc in the numerical implementation, the domain is slightly reduced to $e(t_i) + \varepsilon \leq \eta_i \leq d(t_i) - \varepsilon$ where $\varepsilon > 0$ is small.

For the inner loop optimization in Case 0, the solution is a cubic polynomial and its coefficients are determined from the boundary conditions by solving a system of four linear algebraic equations. In Cases 1 and 2, the cubic spline in $[t_i, t_{i+1}]$ consist of two pieces adjoined at the touching point $t_i < \tau_{i,1} < t_{i+1}$. The boundary conditions of (21) and (22), the conditions that $f(\tau_{i,1}), f'(\tau_{i,1})$ match the corresponding values of the constraint and its derivative, and the condition for the continuity of the second derivative of the solution yield a cubic equation for the location of the touching point $\tau_{i,1}$ and eight linear algebraic equations that determine the coefficients of the two cubic polynomials which constitute the cubic spline. Thus in Cases 1 and 2, up to three solution candidates corresponding to the roots of the cubic polynomial need to be considered. The cubic spline with the subarc in Cases 3 and 4 consist of two cubic polynomials adjoining a linear function from both sides. The equations for the ends of the subarc $\tau_{i,1}, \tau_{i,2}$ and for the coefficients of two cubic polynomials are constructed similarly; they reduce to a system of linear algebraic equations. For Cases 5 and 6, determining the location of the two additional knots ($\tau_{i,1}$ and $\tau_{i,2}$) reduces to solving two (coupled) multivariate polynomial equations of order five; then the coefficients of the three cubic polynomials are determined by solving a system of linear algebraic equations. For the former, numerical methods are used. In MATLAB, the options are either `fsolve` that uses Newton's method or `vpasolve` which uses both symbolic and numerical manipulations. In the former case, multiple starting points may need to be used to reliably determine all solution candidates (this is implemented in the function `ic_search` of our codebase). While `vpasolve` is able to reliably find solutions, its run time is about 50 times slower than `fsolve`without `ic_search`. A potential alternative solution, that we leave to future work, is to train a neural network offline to compute the locations of additional knots in the touching pair given problem data in (t_i, t_{i+1}) as inputs. Typically, many of the solution candidates are discarded as they do not satisfy the constraints (this check reduces to finding minima of a cubic function) or the conditions informing each Case.

In the outer loop the function φ is minimized. This function is strictly convex and Lipschitz continuous but may be nonsmooth. In MATLAB, `fminsearch` function is available which implements the Nelder–Mead's method which does not rely on the use of the gradient information. The alternative is the use of the function `fmincon` which is intended for smooth problems, but as it relies only on function values for the computations, it can be applied to minimizing our function. Our numerical experiments indicated that `fminsearch` gives a larger cost solution as compared to `fmincon` and, furthermore, with `fminsearch` the second derivative of the solution is not continuous. In addition, `fminsearch` is slower than `fmincon`. Hence our final implementation uses `fmincon`. A plethora of computational methods for nonsmooth optimization exist[19] which could be alternatively used.

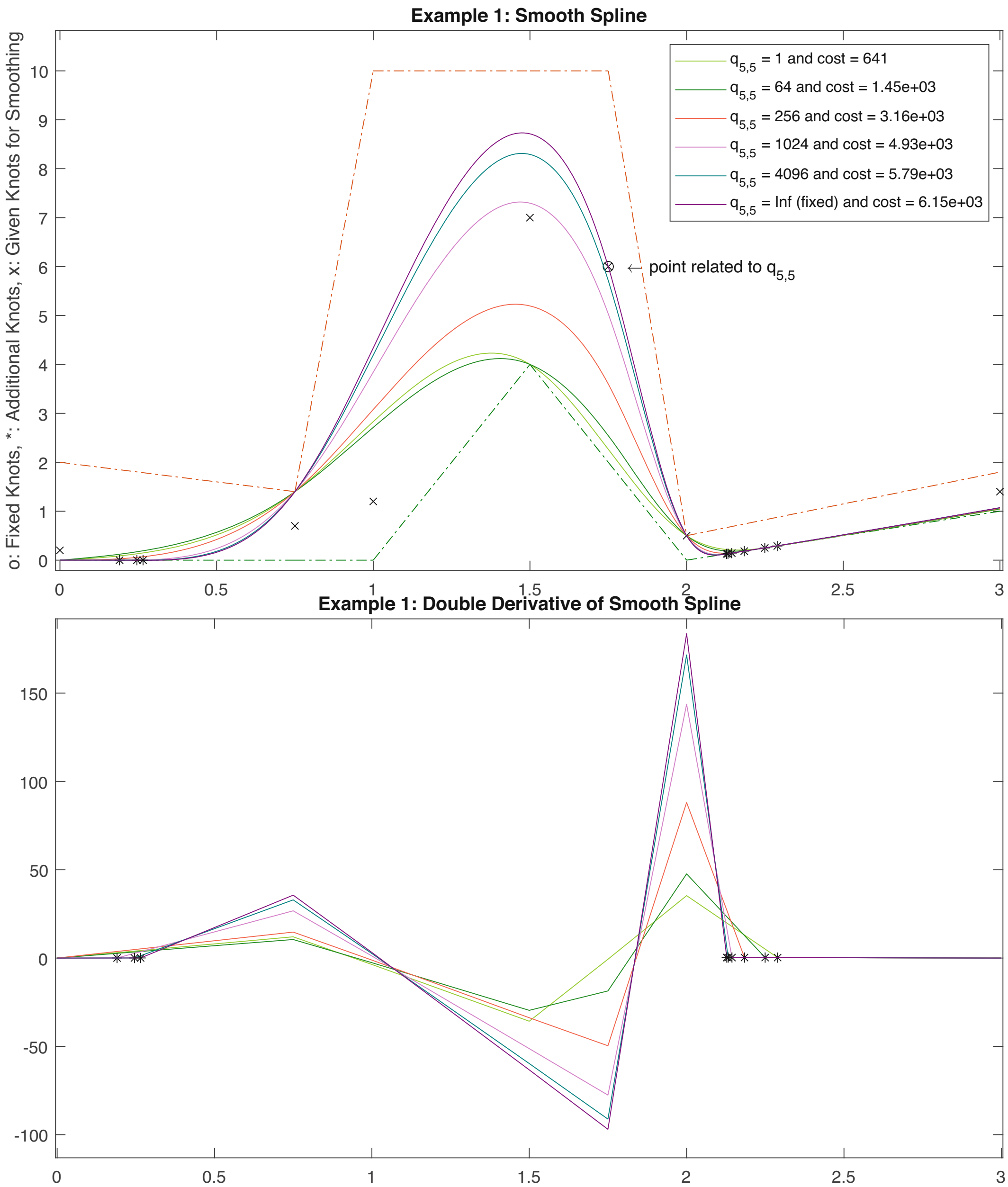

FIGURE 1 Top: The solution as $q_{5,5}$ varies in the first example. Bottom: The second derivative of the solution

Two numerical examples are reported in Figures 1 and 2. In these examples, the starting point (η^0, θ^0) for the outer-loop optimization was set so that

$$\eta_i^0 = 0.5(e(t_i) + d(t_i)), \quad \theta_i^0 = 0, \ i = 1, \ldots, N+2.$$

Both examples were defined on an interval different from $[0, 1]$ (originally assumed in our analysis) in order to illustrate a more general situation. In the first example, the interval is $[t_1, t_{N+2}] = [0, 3]$ and $N = 5$ (7 data points). In the second example, the interval is $[t_1, t_{N+2}] = [13, 25]$ and $N = 4$ (6 data points). The constraints e and d are indicated by the dashed lines in Figures 1 and 2.

In the examples the matrix Q coincides with the identity matrix except for one diagonal element which is varied to illustrate the effects of increasing/decreasing the weight corresponding to a given data point; when this weight is set to ∞ it means that η_j is fixed at y_j and not adjusted in the outer loop optimization (i.e., we replace smoothing by an interpolation

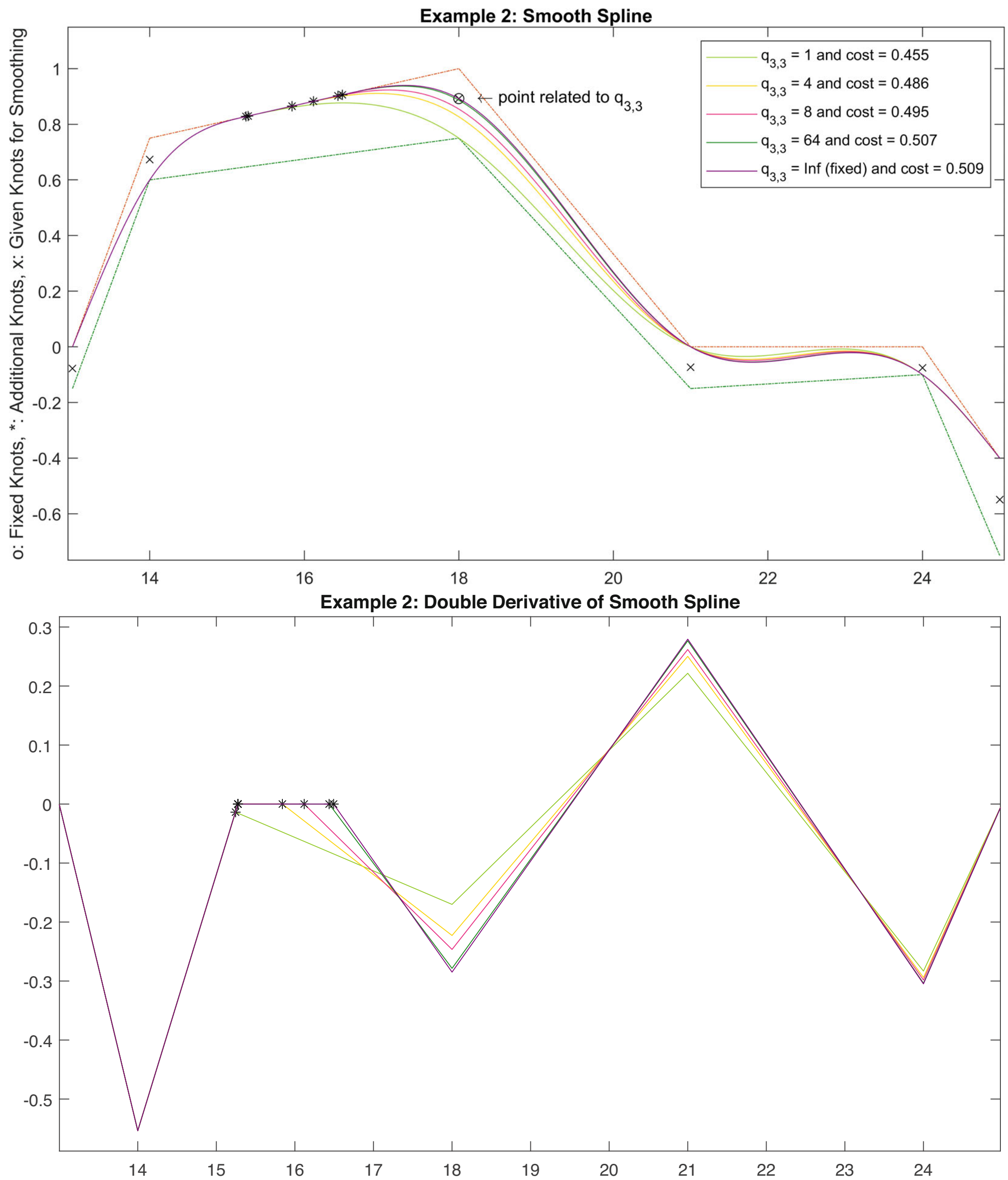

FIGURE 2 Top: The solution as $q_{3,3}$ varies in the second example. Bottom: The corresponding second derivative

constraint at that specific point). Such η_j is indicated by "o" in Figures 1 and 2. In the first example $q_{5,5}$ is varied and in the second example $q_{3,3}$ is varied. The increase in the weight causes the solution to approach closer the specified data point.

The locations of y_i are indicated by "x" in Figures 1 and 2 and the additional knots in each interval (t_i, t_{i+1}) are indicated by "*." To avoid excessive annotation, the knots located at the intervals' starting and ending points (t_i's) are not marked.

Note that the second derivative of the constructed solution is continuous and piecewise linear in both examples, and that the second derivative being zero at t_1 and t_{N+2} is consistent with our theoretical results.

The computations were carried out on a Lenovo Legion Y520 computer with 16 GB of RAM and an Intel Core i7-7700HQ 2.80 GHz processor. When `fsolve` without `ic_search` was used, the runtime was several minutes of calculation. This run time could be improved by warm starting (e.g., from an unconstrained interpolating cubic spline).

Remark 1. As an alternative approach to our problem, we could consider a discretized approximation of the original problem. Specifically, suppose we discretize the interval $[t_0, t_{N+2}]$ into m equally spaced sub-intervals, where $m \gg N + 2$, with the sub-interval end points being $\{\tau_k\}_{k=0}^{m}$. Then we could consider two strategies.

The first and fairly standard strategy would be to treat u as a constant in interval $[\tau_k, \tau_{k+1}]$ and only impose constraints on x_1 at τ_k's. The problem with this formulation is that u is piecewise constant and may not be not continuous, which is not consistent with our theoretical results derived for the original infinite-dimensional optimization problem. Specifically, we know that the optimal u must be continuous on $[t_0, t_{N+2}]$ and satisfy $u(t_0) = u(t_{N+2}) = 0$. The second formulation tries to address this by treating the third derivative $v = \dddot{x}_1$ of x_1 as constant in each sub-interval $[\tau_k, \tau_{k+1}[$; similarly, we only impose the constraints on x_1 at τ_k's.

It can be easily shown that both discretized approximation approaches reduce to quadratic programming (QP) problems. Such problems can then be solved using QP solvers.

The main issue with the above discretized approximation approaches is that the constraints are only imposed and enforced at the points, τ_k. Hence, unlike with the approach proposed in this article, "intersample" constraint violations could occur. Additionally, the QP problem can be large-dimensional and not trivial to solve if fine discretization is used. At the same time, if the QP problem could be solved cheaply (e.g., for not very fine discretization) then an approximate solution through the discretization and QP could be of use for warm-starting, that is, for providing an initial guess to both the outer loop and the inner loop optimizers described in this article. We leave the comprehensive investigation of potential synergies between the approach in this article and alternative approaches based on discretization and QP to a future publication.

6 | CONCLUSIONS

In this article we considered a problem of best smoothing in a strip and connected this problem to a state-constrained optimal control problem for the double integrator. Conditions for the existence and uniqueness of the solution were given under which the solution was shown to be a cubic spline with no more than two additional knots in each interval between the given data points. A numerical algorithm for solving this problem based on a two stage minimization was proposed; its efficacy was illustrated using numerical examples.

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DATA AVAILABILITY STATEMENT

The data that support the findings of this study are openly available in the *Best Interpolation and Data Smoothing in a Strip* repository at https://gitlab.eecs.umich.edu/trungbt/best-interpolation-in-a-strip, Reference number 20. The numerical examples can be found in the `\plots\Case Study II` folder in the codebase.

ENDNOTE

*This follows since L_2-squared norm is strictly convex, $\tilde{Q} \succ 0$, $Q \succcurlyeq 0$ and noting that $u = \ddot{x}_1^{(1)} = \ddot{x}_1^{(2)}$, $x_1^{(1)}(t_i) = x_1^{(2)}(t_i)$, $x_1^{(1)}(t_j) = x_1^{(2)}(t_j)$ imply that $x_1^{(1)}(t) = x_1^{(2)}(t)$ for all $0 \leq t \leq 1$. The full details of the proof are analogous to the ones of strict convexity of the function φ in Section 4; we chose not to repeat them here.

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