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A Constrained Optimal Control Approach to Smoothing Splines

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***Abstract*— This paper addresses smoothing spline estimation of complex functions subject to shape and/or dynamics constraints. Such estimation problems receive growing interest in engineering and statistics, particularly newly emerging areas such as systems biology. In this paper, we formulate the estimation problem as an optimal control problem subject to convex control constraints. By exploring techniques from convex and variational analysis, the existence and uniqueness of optimal solutions is established and explicit optimality conditions are obtained. It is shown that the optimality conditions are given in term of a two-point boundary value problem for a complementarity system. To compute an optimal solution, we formulate the optimality conditions as a B-differentiable equation. A nonsmooth Newton's method is exploited to solve this equation; global convergence of this method is established.**

I. Introduction

Spline models are extensively studied in approximation theory, numerical analysis, and statistics with broad applications in diverse fields. Informally speaking, a univariate spline model provides a piecewise polynomial curve that "best" fits a given finite set of data. Such a spline can be attained via efficient numerical algorithms and enjoys many favorable analytic and statistical properties. A number of variations and extensions have been developed, for example, penalized polynomial splines [14] (simply P-splines) and smoothing splines [18]. In particular, the smoothing spline model is to find a smooth function $f : [0,1] \to \mathbb{R}$ in a suitable function space that minimizes the following objective functional:

$$\frac{1}{n}\sum_{i=1}^{n}\big(f(t_i)-y_i\big)^2+\lambda^*\int_0^1\Big(f^{(m)}(t)\Big)^2dt, \qquad (1)$$

where y_i are noisy data at points $t_i \in [0,1], i = 1,\dots,n$, $f^{(m)}$ denotes the m-th derivative of f, and $\lambda^* > 0$ is a penalty parameter that characterizes a tradeoff between data fidelity and smoothness of f. We refer the interested reader to [18] and the references therein for extensive discussions on statistical properties of smoothing splines.

From a control system point of view, the smoothing spline model (1) is closely related to the linear quadratic optimal control problem by treating $f^{(m)}$ as a control input [3]. This observation has led to a highly interesting spline model, which the authors of [3] coined as *control theoretic splines*. It is shown in [3] and the references therein, e.g. [16], [19], [20], that a variety of smoothing, interpolation, and path planning problems can be modeled in such the paradigm and studied via control theory and optimization techniques on Hilbert spaces with efficient numerical schemes. Other relevant references include control theoretic wavelets [5].

In spite of the significant progress mentioned above, most spline literature deals with *unconstrained* functions. However, various models of biological, engineering and economic systems contain functions whose shape and/or dynamics are subject to inequality constraints, e.g., the monotone and convex constraints. For example, regulatory functions in genetic networks are monotone [15]; another example is the shape restricted function in an attitude control system with the constraint $f^{(3)} \geq 0$ [11]. Incorporating the knowledge of constraints into an estimation procedure is beneficial, since it improves estimation efficiency and accuracy [10]. Two classes of constraints usually arise in the framework of linear optimal control for smoothing splines: (i) control constraints; and (ii) state constraints. Being more tractable, (general) control constraints remain posing many critical open issues in analysis and computation, due to the nonsmooth nature of the problem. Furthermore, many shape constraints are imposed on derivatives of a function and can be formulated as control constraints. Motivated by this, we develop optimality conditions for a class of smoothing splines with convex control constraints using optimal control and optimization techniques in this paper. The resulting optimality conditions lead to a two-point boundary-value problem of complementarity systems [12], [13]. While certain special cases, e.g., the monotone case, have been addressed in [3], [7], [17], [21], [22], general control constraints have not been studied yet. The latter are treated in a unified framework in this paper. The obtained results form a cornerstone for investigation of statistical properties of the splines.

The paper is organized as follows. In Section II, we formulate the smoothing spline as an optimal control problem subject to control constraints. Detailed development of optimality conditions are given in Section III. Section IV addresses numerical issues of the smoothing splines.

II. Problem Formulation

Consider the following (generalized) regression problem on the interval $[0,1]$:

$$y_i \,=\, f(t_i)+\varepsilon_i, \qquad i=1,\dots,n, \qquad (2)$$

where t_i's are the pre-specified design points with $0 < t_1 < \cdots < t_n < 1$, y_i's are samples, ε_i are random noise, and the underlying function $f : [0,1] \to \mathbb{R}$ is assumed to satisfy

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$f(t) = c^T x(t)$, where $c \in \mathbb{R}^\ell$ is given, and $x : [0, 1] \to \mathbb{R}^\ell$ is a vector-valued absolutely continuous function satisfying the following linear differential equation:

$$\dot{x}(t) = Ax(t) + bu(t), \quad \text{a.e. } [0, 1], \tag{3}$$

subject to the control constraint:

$$u(t) \in \Omega, \quad \forall\ t \in [0, 1], \tag{4}$$

where $A \in \mathbb{R}^{\ell \times \ell}$ and $b \in \mathbb{R}^\ell$ are known, and $u \in L_2[0, 1]$. Here $\Omega \subseteq \mathbb{R}$ is a closed convex constraint set, and $L_2[0, 1]$ is the space of (Lebesgue) square integrable functions, endowed with the inner product $\langle v, w\rangle_2 := \int_0^1 v(t)w(t)dt$ for $v, w \in L_2[0, 1]$ and the induced norm $\| \cdot \|_{L_2}$. Since u in (3) can be viewed as the control input to the linear system (3), Ω can be treated as the control constraint.

In summary, the generalized smoothing spline estimator is $c^T x(t)$ with an absolutely continuous $x(t)$ which minimizes the functional

$$J := \sum_{i=1}^n \big(y_i - c^T x(t_i)\big)^2 + \alpha \int_0^1 u^2(t)dt, \tag{5}$$

subject to the dynamics and control constraints (3)-(4), where $\alpha := n\lambda^* > 0$ is the penalty parameter.

Example 2.1: The above model covers a wide range of estimation problems subject to shape and/or dynamical constraints. For instance, the standard monotone regression problem is a special case where $A = 0$, $c = b = 1$ and $\Omega = \mathbb{R}_+$. Another case is the convex regression, for which

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad b = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad c = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \Omega = \mathbb{R}_+.$$

III. Optimality Conditions of Constrained Smoothing Splines

In this section, we establish optimality conditions for the constrained smoothing splines and discuss its complementarity system formulation.

A. Characterization of optimality conditions

To show the existence and uniqueness of an optimal solution and to establish its characterization conditions, we introduce the following basis functions inspired by [3]:

$$p_i(t) := \begin{cases} c^T e^{A(t_i - t)} b & \text{if } t \in [0, t_i] \\ 0 & \text{if } t > t_i \end{cases}, \quad i = 1, \ldots, n.$$

Hence,

$$f(t_i) = c^T x(t_i) = c^T e^{At_i} x_0 + \int_0^1 p_i(t)u(t)dt, \quad i = 1, \ldots, n,$$

where x_0 denotes the initial state of $x(t)$. The objective functional becomes

$$\begin{aligned} J(u, x_0) \quad = \quad & \sum_{i=1}^n \big(c^T e^{At_i} x_0 + \int_0^1 p_i(t)u(t)dt - y_i\big)^2 \\ & + \alpha \int_0^1 u^2(t)dt. \end{aligned} \tag{6}$$

Letting $\mathcal{W} := \{w \in L_2[0, 1] : w(t) \in \Omega, \forall\ t \in [0, 1]\}$ and $\mathcal{P} := \mathcal{W} \times \mathbb{R}^\ell$, the optimization problem is equivalent to

$$\inf_{(u, x_0) \in \mathcal{P}} J(u, x_0) \tag{7}$$

For given design points $\{t_i\}_{i=1}^n$, define the condition:

$$\mathbf{H}: \quad \text{rank} \begin{bmatrix} c^T e^{At_1}, & c^T e^{At_2}, & \cdots, & c^T e^{At_n} \end{bmatrix}^T = \ell.$$

It is easy to see that if (c^T, A) is an observable pair, then the condition $\mathbf{H}$ holds for all sufficiently large n. Under this condition, the existence and uniqueness of an optimal solution can be shown via standard arguments in functional analysis, e.g., [1], [6]. We present its proof in the following theorem for self-containment.

Theorem 3.1: Given $\{t_i\}, \{y_i\}$ and $\alpha > 0$. Under the condition $\mathbf{H}$, the optimization problem (7) has a unique optimal solution $(u^*, x_0^*) \in \mathcal{P}$.

Proof: Consider the Hilbert space $L_2[0, 1] \times \mathbb{R}^\ell$ endowed with the inner product $\langle (u, x), (v, z)\rangle := \int_0^1 u(t)v(t)dt + x^T z$ for any $(u, x), (v, z) \in L_2[0, 1] \times \mathbb{R}^\ell$. Its induced norm $\|(u, x)\|^2 := \|u(t)\|_{L_2}^2 + \|x\|^2$, where the latter $\| \cdot \|$ is a vector norm on $\mathbb{R}^\ell$. We first show that the objective functional $J : L_2[0, 1] \times \mathbb{R}^\ell \to \mathbb{R}$ is coercive, i.e., for any sequence (u_k, x_k) with $\|(u_k, x_k)\| \to \infty$ as $k \to \infty$, $J(u_k, x_k) \to \infty$. Consider two cases: (i) $\|u_k\|_{L_2} \to \infty$ as $k \to \infty$; (ii) otherwise. The first case is trivial in view of the expression of $J(u, x_0)$ in (6). For the second case where $\|u_k\|_{L_2}$ is bounded and $\|x_k\| \to \infty$ as $k \to \infty$, let $Q := \sum_{i=1}^n (c^T e^{At_i})^T (c^T e^{At_i}) \in \mathbb{R}^{\ell \times \ell}$ which is symmetric and positive definite under the condition $\mathbf{H}$. It is noted that

$$\begin{aligned} & J(u_k, x_k) \\ & = x_k^T Q x_k + 2 \sum_{i=1}^n c^T e^{At_i} x_k \big(\int_0^1 p_i(t)u_k(t)dt - y_i \big) \\ & \quad + \sum_{i=1}^n \big(\int_0^1 p_i(t)u_k(t)dt - y_i \big)^2 + \alpha \int_0^1 u_k^2(t)dt \\ & \geq \sqrt{\lambda_{\min}(Q)} \|x_k\|^2 \\ & \quad - 2\|x_k\| \cdot \sum_{i=1}^n \big| \int_0^1 p_i(t)u_k(t)dt - y_i \big| \cdot \|e^{A^T t_i} c\| \\ & \geq \|x_k\| \big(\sqrt{\lambda_{\min}(Q)} \|x_k\| - M \big), \end{aligned}$$

where $\lambda_{\min}(Q)$ is the smallest positive eigenvalue of Q and the bound $M \geq 0$ is due to the boundedness of $\|u_k\|_{L_2}$. Hence $J(u_k(t), x_k) \to \infty$ as $k \to \infty$.

Next we show that $J(u, x_0)$ is strictly convex on $L_2[0, 1] \times \mathbb{R}^\ell$, i.e., for any $(u, x), (v, z) \in L_2[0, 1] \times \mathbb{R}^\ell$ with $(u, x) \neq (v, z)$, $J(\lambda(u, x) + (1 - \lambda)(v, z)) < \lambda J(u, x) + (1 - \lambda)J(v, z)$ for all $\lambda \in (0, 1)$. Given $(u, x), (v, z)$ with $(u, x) \neq (v, z)$, consider two cases: (i) $u \neq v$ (i.e. v is not in the equivalent class of u or $\|u - v\|_{L_2} \neq 0$); (ii) otherwise. To handle this, we use the fact that for any reals $a \neq b$, $[\lambda a + (1 - \lambda)b]^2 < \lambda a^2 + (1 - \lambda)b^2, \forall\ \lambda \in (0, 1)$. For the first case, we have $J(\lambda(u, x) + (1 - \lambda)(v, z)) < \lambda J(u, x) + (1 - \lambda)J(v, z)$, for all $\lambda \in (0, 1)$, where the above strict inequality is due to the observation that the summation on the right satisfies the non-strict inequality but the integral term satisfies the strict inequality. In the second case where $\|u-v\|_{L_2}=0$ and $x \neq z$, we have

$$\begin{aligned} & J(\lambda(u,x)+(1-\lambda)(v,z)) \\ &= [\lambda x+(1-\lambda)z]^T Q[\lambda x+(1-\lambda)z] \\ &\quad +2\sum_{i=1}^{n}\big(c^T e^{At_i}[\lambda x+(1-\lambda)z] \\ &\quad +\int_0^1 p_i(t)[\lambda u(t)+(1-\lambda)v(t)]dt-y_i\big) \\ &\quad +\alpha\int_0^1[\lambda u(t)+(1-\lambda)v(t)]^2 dt. \end{aligned}$$

Since Q is positive definite and $x \neq z$, $[\lambda x+(1-\lambda)z]^T Q[\lambda x+(1-\lambda)z] < \lambda x^T Qx+(1-\lambda)z^T Qz$ for all $\lambda \in (0,1)$. Furthermore, since $\|u-v\|_{L_2}=0$,

$$\begin{aligned} & \sum_{i=1}^{n}\big(c^T e^{At_i}[\lambda x+(1-\lambda)z] \\ &\qquad +\int_0^1 p_i(t)[\lambda u(t)+(1-\lambda)v(t)]dt-y_i\big) \\ &= \lambda\sum_{i=1}^{n}\big(c^T e^{At_i}x+\int_0^1 p_i(t)u(t)dt-y_i\big) \\ &\qquad +(1-\lambda)\sum_{i=1}^{n}\big(c^T e^{At_i}z+\int_0^1 p_i(t)v(t)dt-y_i\big), \end{aligned}$$

and $\int_0^1[\lambda u(t)+(1-\lambda)v(t)]^2dt \leq \lambda\int_0^1 u^2(t)dt+(1-\lambda)\int_0^1 v^2(t)dt$. Thus $J(\lambda(u,x)+(1-\lambda)(v,z)) < \lambda J(u,x)+(1-\lambda)J(v,z), \forall\, \lambda \in (0,1)$, i.e., J is strictly convex.

Pick an arbitrary $(\widetilde{u},\widetilde{x}) \in \mathcal{P}$ and define the level set $\mathcal{S} := \{(u,x) \in \mathcal{P} : J(u,x) \leq J(\widetilde{u},\widetilde{x})\}$. Due to the convexity and the coercive property of J, $\mathcal{S}$ is a convex and (L_2-norm) bounded set in $L_2[0,1]\times\mathbb{R}^\ell$. Since the space $L_2[0,1]\times\mathbb{R}^\ell$ is reflexive and self dual, it follows from Banach-Alaoglu Theorem [6] that an arbitrary sequence $\{(u_n,x_n)\}$ in $\mathcal{S}$ has a subsequence $\{(u'_n,x'_n)\}$ that attains a weak*, thus weak, limit $(u^*,x^*) \in L_2[0,1]\times\mathbb{R}^\ell$. Therefore, $c^T e^{At_i}x'_n+\int_0^1 p_i(t)u'_n(t)dt$ converges to $c^T e^{At_i}x^*+\int_0^1 p_i(t)u^*(t)dt$ for each i. Further, by using the (L_2-norm) boundedness of $\{u'_n\}$ and the triangle inequality for the L_2-norm, it is easy to show that for any $\eta > 0$, there exists $K \in \mathbb{N}$ such that $\|u^*\|^2_{L_2} \leq \|u'_n\|^2_{L_2}+\eta, \forall\, n \geq K$. These results imply that for any $\varepsilon > 0$, $J(u^*,x^*) \leq J(u'_n,x'_n)+\varepsilon$ for all n sufficiently large. Consequently, $J(u^*,x^*) \leq J(\widetilde{u},\widetilde{x})$ such that $(u^*(,x^*) \in \mathcal{S}$. This thus shows that $\mathcal{S}$ is weakly compact. In view of (strong) continuity of J, we see that a global optimal solution exists on $\mathcal{S}$ [6, Section 5.10, Theorem 2], and thus on $\mathcal{P}$. Further, since J is strictly convex and the set $\mathcal{P}$ is convex, there is a unique optimal solution. ■

The next result provides the necessary and sufficient optimality conditions in terms of variational inequalities.

Theorem 3.2: The pair $(u^*,x_0^*) \in \mathcal{P}$ is an optimal solution to (7) if and only if the following two conditions hold:

$$\begin{aligned} & \Big(v(t)-u^*(t)\Big)\Big[\alpha u^*(t)+\sum_{i=1}^{n}\big(c^T e^{At_i}x_0^* \\ &\qquad +\int_0^1 p_i(t)u^*(t)dt-y_i\big)p_i(t)\Big] \geq 0, \ \text{a.e.}[0,1], \quad (8) \end{aligned}$$

$\forall\ v \in \mathcal{W}$, and

$$\sum_{i=1}^{n}\Big(c^T e^{At_i}x_0^*+\int_0^1 p_i(t)u^*(t)dt-y_i\Big)c^T e^{At_i}=0. \quad (9)$$

Proof: Let $(u',x') \in \mathcal{P}$ be arbitrary. Due to the convexity of $\mathcal{P}$, $(u^*,x_0^*)+\varepsilon[(u',x')-(u^*,x_0^*)] \in \mathcal{P}$ for all $\varepsilon \in [0,1]$. Further, since (u^*,x_0^*) is a global optimizer, we have $J((u^*,x_0^*)+\varepsilon[(u',x')-(u^*,x_0^*)]) \geq J(u^*,x_0^*)$ for all $\varepsilon \in [0,1]$. Therefore

$$\begin{aligned} 0 &\leq \lim_{\varepsilon\downarrow 0}\frac{J((u^*,x_0^*)+\varepsilon[(u',x')-(u^*,x_0^*)])-J(u^*,x_0^*)}{\varepsilon} \\ &= 2\Big[\sum_{i=1}^{n}\big(c^T e^{At_i}x_0^*+\int_0^1 p_i(t)u^*(t)dt-y_i\big) \\ &\qquad \big(c^T e^{At_i}(x'-x_0^*)+\int_0^1 p_i(t)(u'(t)-u^*(t))dt\big) \\ &\qquad +\alpha\int_0^1 u^*(t)(u'(t)-u^*(t))dt\Big]. \end{aligned}$$

This thus yields the necessary optimality condition: for all $(u',x') \in \mathcal{P}$,

$$\begin{aligned} & \sum_{i=1}^{n}\Big(c^T e^{At_i}x_0^*+\int_0^1 p_i(t)u^*(t)dt-y_i\Big) \\ &\qquad \Big[c^T e^{At_i}(x'-x_0^*)+\int_0^1 p_i(t)(u'(t)-u^*(t))dt\Big] \\ &\qquad +\alpha\int_0^1 u^*(t)(u'(t)-u^*(t))dt \geq 0. \end{aligned}$$

This condition is also sufficient in light of the following inequality due to the convexity of J:

$$\begin{aligned} & J(u',x')-J(u^*,x_0^*) \\ &\quad \geq \lim_{\varepsilon\downarrow 0}\frac{J((u^*,x_0^*)+\varepsilon[(u',x')-(u^*,x_0^*)])-J(u^*,x_0^*)}{\varepsilon}, \end{aligned}$$

$\forall\ (u',x') \in \mathcal{P}$. Noticing that x' is arbitrary in the vector space $\mathbb{R}^\ell$, it is easy to show (by setting $u'(t)=u^*(t)$) that the terms before $x'-x_0^*$ must be zero. This yields the equivalent condition (9) and

$$\int_0^1\Big(u'(t)-u^*(t)\Big)H(u^*(t),x_0^*)dt \geq 0,$$

where $H(u^*(t),x_0^*) := \alpha u^*(t)+\sum_{i=1}^{n}\big(c^T e^{At_i}x_0^*+\int_0^1 p_i(t)u^*(t)dt-y_i\big)p_i(t)$, for all $u' \in L_2[0,1]$ with $u' : [0,1] \to \Omega$. Since $H(u^*,x_0^*) \in L_2[0,1]$ and $u' \in L_2[0,1]$, it follows from [9, Section 2.1] that the above integral inequality is equivalent to the variational inequality (8). ■

Recall that the control constraint Ω is a closed convex subset of $\mathbb{R}$. Hence, Ω must be an interval of one of the following types: (1) $\Omega=[\mu_1,\infty)$; (2) $\Omega=(-\infty,\mu_2]$; and

(3) $\Omega = [\mu_1, \mu_2]$ with $\mu_1 < \mu_2$, where $\mu_1, \mu_2 \in \mathbb{R}$. (Here we omit the trivial case $\Omega = \mathbb{R}$.) This allows us to simplify the variational inequality (8) using complementarity formulation. In the following, let $x^*(t) := e^{At}x_0^* + \int_0^t e^{A(t-s)}bu^*(s)ds$ and let $\widehat{f}(t) := c^T x^*(t)$ be the smoothing spline estimator.

Proposition 3.1: The following hold:

(1) If $\Omega = [\mu_1, \infty)$, then (8) is equivalent to a.e. $[0, 1]$,

$$u^*(t) = \Big[-\mu_1 - \alpha^{-1} \sum_{i=1}^n \big(\widehat{f}(t_i) - y_i\big)p_i(t)\Big]_+ + \mu_1;$$

(2) If $\Omega = (-\infty, \mu_2]$, then (8) is equivalent to a.e. $[0, 1]$,

$$u^*(t) = \mu_2 - \Big[\mu_2 + \alpha^{-1} \sum_{i=1}^n \big(\widehat{f}(t_i) - y_i\big)p_i(t)\Big]_+;$$

(3) If $\Omega = [\mu_1, \mu_2]$ with $\mu_1 < \mu_2$, then (8) is equivalent to a.e. $[0, 1]$,

$$u^*(t) = \text{sat}\Big(\sum_{i=1}^n \big(\widehat{f}(t_i) - y_i\big)p_i(t)\Big),$$

where $\text{sat}(\cdot)$ denotes the following saturation function defined by:

$$\text{sat}(z) := \begin{cases} \mu_2, & \text{if } z \le -\alpha\mu_2 \\ -\alpha^{-1}z, & \text{if } z \in [-\alpha\mu_2, -\alpha\mu_1] \\ \mu_1, & \text{if } z \ge -\alpha\mu_1 \end{cases} \tag{10}$$

Proof: For notational simplicity, let $g(u^*(t), x_0^*) := \sum_{i=1}^n \big(c^T e^{At_i} x_0^* + \int_0^1 p_i(t)u^*(t)dt - y_i\big)p_i(t) = \sum_{i=1}^n \big(\widehat{f}(t_i) - y_i\big)p_i(t)$. Hence the variational inequality (8) becomes $\big(v - u^*(t)\big)\big[\alpha u^*(t) + g(u^*(t), x_0^*)\big] \ge 0$, a.e. $[0, 1]$ for all $v \in \mathcal{W}$. Since each Ω is a linear (i.e. polyhedral) constraint, it follows from [2, Lemma 5.1.4] that the Abadie's Constraint Qualification holds such that the variational inequality (8) can be equivalently described by the following Karush-Kuhn-Tucker (KKT) conditions [4, Proposition 1.3.4]:

(1) $\Omega = [\mu_1, \infty)$. In this case, $\Omega = \{v \in \mathbb{R} : v - \mu_1 \ge 0\}$ and the corresponding KKT conditions are:

$$\alpha u^*(t) + g(u^*(t), x_0^*) - \chi = 0, \qquad 0 \le \chi \perp u^*(t) - \mu_1 \ge 0,$$

where $a \perp b$ means two objects are orthogonal, i.e. $a^T b = 0$. Letting $v^*(t) := u^*(t) - \mu_1$, the KKT conditions become

$$0 \le \alpha v^*(t) + \alpha\mu_1 + g(u^*(t), x_0^*) \perp v^*(t) \ge 0.$$

This is equivalent to $\alpha v^*(t) = \big[-\alpha\mu_1 - g(u^*(t), x_0^*)\big]_+$ which leads to the desired condition.

(2) $\Omega = (-\infty, \mu_2]$. This case is similar to the first one and its development is omitted.

(3) $\Omega = [\mu_1, \mu_2]$ with $\mu_1 < \mu_2$. Here $\Omega = \{v \in \mathbb{R} : Ev - d \ge 0\}$, where $E = [1, -1]^T$ and $d = [\mu_1, -\mu_2]^T$. (The inequality $\ge$ holds componentwise.) The corresponding KKT conditions are:

$$\alpha u^*(t) + g(u^*(t), x_0^*) - E^T\chi = 0$$

and $0 \le \chi \perp Eu^*(t) - d \ge 0$, where $\chi = [\chi_1, \chi_2]^T \in \mathbb{R}^2$. This is equivalent to

$$0 \le \chi \perp (n\alpha)^{-1}EE^T\chi - (n\alpha)^{-1}Ez - d \ge 0,$$

where $z \equiv g(u^*(t), x_0^*)$. It is known from complementarity theory that $E^T\chi$ in the above complementarity problem is unique for any $z \in \mathbb{R}$ and is indeed a continuous piecewise affine function of z given by:

$$E^T\chi(z) = \begin{cases} \alpha\mu_2 + z, & \text{if } z \le -\alpha\mu_2 \\ 0, & \text{if } z \in [-\alpha\mu_2, -\alpha\mu_1] \\ \alpha\mu_1 + z, & \text{if } z \ge -\alpha\mu_1 \end{cases} \tag{11}$$

Therefore $u^*(t) = (\alpha)^{-1}[-g(u^*(t), x_0^*) + E^T\chi(g(u^*(t), x_0^*))] = \text{sat}(g(u^*(t), x_0^*))$. ■

An interesting special case is when A is the following nilpotent matrix:

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ & & \ddots & \ddots & & \vdots \\ 0 & \cdots & 0 & 0 & 1 & 0 \\ 0 & \cdots & 0 & 0 & 0 & 1 \\ 0 & \cdots & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{12}$$

In this case, each component of e^{At} is a polynomial, i.e.

$$e^{At} = \begin{bmatrix} 1 & t & \frac{t^2}{2!} & \frac{t^3}{3!} & \cdots & \frac{t^{(\ell-1)}}{(\ell-1)!} \\ 0 & 1 & t & \frac{t^2}{2!} & \cdots & \frac{t^{(\ell-2)}}{(\ell-2)!} \\ & & \ddots & \ddots & & \vdots \\ 0 & \cdots & 0 & 1 & t & \frac{t^2}{2!} \\ 0 & \cdots & 0 & 0 & 1 & t \\ 0 & \cdots & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Therefore, each $p_i(t)$ is a (possibly discontinuous) piecewise polynomial on $[0, 1]$. In fact, if $c^T b = 0$, then $p_i(t)$ is continuous on $[0, 1]$; otherwise, $p_i(t)$ is only discontinuous at t_i. In view of this, Proposition 3.1 and the fact that both the plus function $(\cdot)_+$ and the saturation function in (10) are continuous and piecewise linear or affine, we thus have:

Corollary 3.1: If A is the nilpotent matrix given in (12), then $u^*(t)$ is a (possibly discontinuous) piecewise polynomial on $[0, 1]$. Further, each element of $x(t)$ is an absolutely continuous piecewise polynomial on $[0, 1]$.

Due to the presence of the dynamics (characterized by A) and the control constraint, the degree change of polynomials in $u^*(t)$ occurs not only at points t_i but also possibly between two consecutive points. This is different from the classical unconstrained splines.

Remark 3.1: The above optimality results can be extended to a linear time-varying system of the form $\dot{x}(t) = A(t)x(t) + b(t)u(t)$ and $f(t) = c^T(t)x(t)$, where $A : [0, 1] \to \mathbb{R}^{\ell \times \ell}$ and $b, c : [0, 1] \to \mathbb{R}^\ell$ are piecewise continuous.

B. Characterization via complementarity systems

Recall that $x^*(t) = e^{At}x_0^* + \int_0^t e^{A(t-s)}bu^*(s)ds$ and $\widehat{f}(t) = c^T x^*(t)$. To characterize the estimator, we make the following assumptions:

A.1 The matrix-vector tuple (A, b, c^T) satisfies $c^T A^k b = 0, \forall\ k = 0, \ldots, \ell-2$, and $c^T A^{\ell-1} b \neq 0$.

A.2 The pair (A, b) is a controllable pair.

Without loss of generality, we may let $c^T A^{\ell-1} b = 1$. Assumption **A.1** implies that the linear control system (A, b, c^T) has the relative degree $(\ell-1)$. Under this assumption, it is easy to show that for each $k = 1, \ldots, \ell$, $\widehat{f}^{(k)}(t)$ exists almost everywhere on $[0,1]$ and is given by

$$\widehat{f}^{(k)}(t) = \begin{cases} c^T A^k x^*(t), & \text{if } \ k \leq \ell - 1 \\ c^T A^\ell x^*(t) + c^T A^{\ell-1} b u^*(t), & \text{if } \ k = \ell \end{cases}$$

By the Cayley-Hamilton Theorem, $A^\ell = \sum_{k=0}^{\ell-1} a_k A^i$ for some real numbers a_k. Therefore, $\widehat{f}^{(\ell)}(t) = \sum_{k=0}^{\ell-1} a_k \widehat{f}^{(k)}(t) + u^*(t)$. Furthermore, let ω be the uniform distribution on $\{t_1, \ldots, t_n\}$ and $\mathcal{I}$ denotes the indicator function of a set. For any function $h : [0,1] \to \mathbb{R}$ and $t \in [0,1]$, $\int_0^t h(s) d\omega(s) := \frac{1}{n} \sum_{i=1}^n h(t_i) \mathcal{I}([t_i, 1])$. Hence, $\int_0^t h(s) d\omega(s) = 0$ if $t \in [0, t_1)$ and $\int_0^t h(s) d\omega(s) = \frac{1}{n} \sum_{i=1}^j h(t_i)$ for each $t \in [t_j, t_{j+1})$, $j = 1, \ldots, n-1$. Therefore, for $t \in [0,1]$, $\int_t^1 h(s) d\omega(s) := \frac{1}{n} \sum_{i=1}^n h(t_i) \mathcal{I}([0, t_i])$.

For the given $\{y_i\}$, let $g : [0,1] \to \mathbb{R}$ be the piecewise constant function defined by $\{y_i\}$, namely, $g(t) := 0, \forall\ t \in [0, t_1)$, and $g(t) := y_i, \quad \forall\ t \in [t_i, t_{i+1}), \quad i = 1, \ldots, n-1$. For a function $h : [0,1] \to \mathbb{R}$, define

$$W(h, t) := W_{(0)}(h, t) = \int_0^t h(s) c^T e^{A(s-t)} b \, d\omega(s),$$

and $W_{(k)}(h, t) := \int_0^t h(s) c^T e^{A(s-t)} A^k b \, d\omega(s)$. In view of the optimality condition (9) expressed as $\sum_{i=1}^n (\widehat{f}(t_i) - y_i) c^T e^{A t_i} = 0$, it is easily shown that under the assumption **A.2**, (9) is equivalent to $W_{(k)}(\widehat{f}, 1) = W_{(k)}(g, 1), \ \forall\ k = 0, 1, \ldots, \ell-1$. Moreover, noting that $p_i(t) = c^T e^{A(t_i - t)} b \mathcal{I}([0, t_i])$, we have, for any $t \in [t_j, t_{j+1})$,

$$\begin{aligned} \sum_{i=1}^n \big(\widehat{f}(t_i) - y_i\big) p_i(t) &= \sum_{i=j+1}^n \big(\widehat{f}(t_i) - y_i\big) c^T e^{A(t_i - t)} b \\ &= -n \big(W(\widehat{f}, t) - W(g, t)\big). \end{aligned}$$

Putting the above results together and recalling $\lambda^* = \alpha / n$, we obtain the following differential equation subject to two-point boundary conditions in the integral form as the necessary and sufficient optimality conditions:

Theorem 3.3: Under the condition **H** and the assumptions **A.1**-**A.2**, the necessary and sufficient conditions for the estimator $\widehat{f}(t)$ are:

$$\widehat{f}^{(\ell)}(t) = \sum_{k=0}^{\ell-1} a_k \widehat{f}^{(k)}(t) + u^*(t), \tag{13}$$

where

(i) If $\Omega = [\mu_1, \infty)$, $u^*(t) = \Big[-\mu_1 + (\lambda^*)^{-1} \big(W(\widehat{f}, t) - W(g, t)\big) \Big]_+ + \mu_1, \quad$ a.e. $[0,1]$;

(ii) If $\Omega = (-\infty, \mu_2]$, $u^*(t) = \mu_2 - \Big[\mu_2 - (\lambda^*)^{-1} \big(W(\widehat{f}, t) - W(g, t)\big) \Big]_+, \quad$ a.e. $[0,1]$;

(iii) If $\Omega = [\mu_1, \mu_2]$ with $\mu_1 < \mu_2$, $u^*(t) = \text{sat}\big(nW(g, t) - nW(\widehat{f}, t)\big), \quad$ a.e. $[0,1]$,

subject to the boundary conditions $W_{(k)}(\widehat{f}, 1) = W_{(k)}(g, 1)$ and $W_{(k)}(\widehat{f}, 0) = 0, \ \forall\ k = 0, 1, \ldots, \ell-1$.

Define $\widehat{F}(t) := \int_0^t \widehat{f}(s) c^T e^{A(s-t)} b ds$, where $\widehat{F}(t)$ is similar to $W(\widehat{f}, t)$ except that the Lebesgue measure is used in the former while the uniform distribution is used in the latter. It is easy to show via direct computation that under the assumption **A.1**,

$$\widehat{F}^{(k)}(t) = \int_0^t \widehat{f}(s) c^T e^{A(s-t)} (-A)^k b ds, \ \forall\ k = 0, 1, \ldots, \ell-1.$$

Furthermore, we obtain

$$\begin{aligned} \widehat{F}^{(2\ell)}(t) &= \sum_{j=0}^{\ell-1} [(-1)^{\ell-j} + 1]\, a_j \widehat{F}^{(\ell+2j)}(t) \\ &\quad - \sum_{j=0}^{\ell-1} \sum_{k=0}^{\ell-1} (-1)^{\ell-j} a_j a_k \widehat{F}^{(k+j)}(t) + u^*(t), \end{aligned}$$

where $u^*(t)$ is defined in Theorem 3.3. This yields a complementarity system subject the two-point boundary conditions.

IV. Computation of Constrained Splines

In this section, we discuss computation of optimal solutions based on nonsmooth Newton's methods. Note that to determine an optimal solution, it suffices to find the optimal initial state x_0^*, since once x_0^* is known, u^* and $\widehat{f}$ can be computed recursively as shown below.

A. Computation of the optimal initial state x_0^*

To emphasize the dependence of $\widehat{f}$ and u^* on x_0, we use the notation $\widehat{f}(t, x_0)$ and $u^*(t, x_0)$ as follows. The next lemma shows the B(ouligand)-differentiability of $\widehat{f}$ in x_0 [4].

Lemma 4.1: Given $\{y_i\}$. The function $\widehat{f}(t, x_0)$ is B-differentiable with respect to x_0 for any fixed $t \in [0,1]$.

Proof: We focus on the case when $\Omega = [\mu_1, \infty)$; the other cases can be treated in a similar manner. It follows from the optimality conditions derived from the preceding section that for the given $\{y_i\}$ and a given $x_0 \in \mathbb{R}^2$,

$$\widehat{f}(t, x_0) = c^T e^{At} x_0 + \int_0^t c^T e^{A(t-s)} b u^*(s, x_0) ds, \tag{14}$$

where $u^*(t, x_0) = \mu_1 + \big[-\mu_1 + (\lambda^*)^{-1} \int_0^t (\widehat{f}(s, x_0) - g(s)) c^T e^{A(s-t)} b d\omega(s) \big]_+$. For any given t, it is equivalent to show that $\widehat{f}(t, \cdot)$ is Lipschitz continuous and directionally differentiable [4, Chapter 3]. We use induction on the intervals $[t_k, t_{k+1}]$ to prove this. Let $t \in [0, t_1)$. Then $u^*(t, x_0) = (-\mu_1)_+ + \mu_1 = (\mu_1)_+$, and due to the continuity of $\widehat{f}$ in t, $\widehat{f}(t, x_0) = c^T e^{At} x_0 + (\mu_1)_+ \int_0^t c^T e^{A(t-s)} b ds, \forall\, t \in [0, t_1]$, which is clearly Lipschitz continuous and directionally differentiable, thus B-differentiable, in x_0 for any fixed $t \in [0, t_1]$. Now assume that $\widehat{f}(t, \cdot)$ is B-differentiable for all $t \in [0, t_1] \cup \cdots \cup [t_{k-1}, t_k]$. For $t \in [t_k, t_{k+1})$, note that

$$u^*(t, x_0) = \Big[-\mu_1 + \tfrac{1}{\alpha} \textstyle\sum_{i=1}^k (\widehat{f}(t_i, x_0) - y_i) c^T e^{A(t_i - t)} b \Big]_+ + \mu_1. \tag{15}$$

Algorithm 1 Newton's Method with Line Search [8]

Choose scalars $\beta \in (0,1)$ and $\sigma \in (0, \frac{1}{2})$;
Initialize $k = 0$ and choose an initial vector z^0;
repeat
  $k \leftarrow k+1$;
  Find a direction vector d^k such that $H_{y,n}(z^{k-1}) + H'_{y,n}(z^{k-1}; d^k) = 0$;
  Let m_k be the first nonnegative integer m for which $g(z^{k-1}) - g(z^k + \beta^m d^k) \geq -\sigma \beta^m g'(z^{k-1}; d^k)$;
  Set $z^k \leftarrow z^{k-1} + \beta^{m_k} d^k$;
until $|g(z^k)|$ is sufficiently small
return z^k

Since the function $(\cdot)_+$ and $\widehat{f}(t_i, \cdot), i = 1, \ldots, k$ are B-differentiable, the composition given in $u^*(t, \cdot)$ remains so for all $t \in [t_k, t_{k+1})$. In view of $\widehat{f}(t, x_0) = c^T e^{At} x_0 + \int_0^t c^T e^{A(t-s)} b u^*(s, x_0) ds$ and the continuity of $\widehat{f}$ in t, we deduce the B-differentiability of $\widehat{f}(t, \cdot)\ \forall\, t \in [t_k, t_{k+1}]$. Thus the lemma follows by the induction principle. ■

For the given sample $y := \{y_i\}_{i=1}^n \in \mathbb{R}^n$, define the function $H_{y,n} : \mathbb{R}^\ell \to \mathbb{R}^\ell$ as $H_{y,n}(z) := \big(\sum_{i=1}^n \big(\widehat{f}(t_i, z) - y_i \big) c^T e^{At_i} \big)^T$. By the above lemma, we deduce that $H_{y,n}$ is a vector-valued B-differentiable function and that the condition (9) is equivalent to the B-differentiable equation $H_{y,n}(z) = 0$. Nonsmooth Newton's methods can be applied to solve this equation, and its (unique) solution will be the optimal initial state x_0^* that completely determines the estimator.

To describe a nonsmooth Newton's method, we introduce more notation. The directional derivative of $H_{y,n}(z)$ along a direction vector $d \in \mathbb{R}^\ell$ is defined by $H'_{y,n}(z; d) := \lim_{\tau \downarrow 0} \frac{H_{y,n}(z+\tau d) - H_{y,n}(z)}{\tau}$. Hence, $H'_{y,n}(z; d) = \sum_{i=1}^n \widehat{f}'(t_i, z; d) \big(c^T e^{At_i} \big)^T$, where $\widehat{f}'(t_i, z; d)$ is the directional derivative of $\widehat{f}(t_i, \cdot)$ (its existence is shown in Lemma 4.1). We also define the merit function $g(z) := \frac{1}{2} H^T_{y,n}(z) H_{y,n}(z)$ [8]. It is clear that g is B-differentiable and $g'(z; d) = H^T_{y,n}(z) H'_{y,n}(z; d)$. Using this function, we may apply the nonsmooth Newton's method with line search [8] to solve the equation $H_{y,n}(z) = 0$. To be self-contained, we present its numerical procedure in Algorithm 1.

B. Convergence analysis

To show convergence of the proposed Newton's method, we first establish a boundedness result for level sets defined by $H_{y,n}$. For given y and z^*, define the level set $\mathcal{S}_{z^*} := \{ z \in \mathbb{R}^\ell : \| H_{y,n}(z) \| \leq \| H_{y,n}(z^*) \| \}$. The proofs in this section are omitted due to space limitation.

Proposition 4.1: The following statements hold: (1) Let $\Omega = [\mu_1, \mu_2]$ with $\mu_1 < \mu_2$. Then for any $y \in \mathbb{R}^n$ and any given $z^* \in \mathbb{R}^\ell$, the level set $\mathcal{S}_{z^*}$ is bounded.

(2) Let $\Omega = [\mu, \infty)$ or $\Omega = (-\infty, \mu]$. Suppose $\limsup_{n\to\infty} n\alpha^{-1} < 4\rho^{-1}$, where $\rho > 0$ depends on (c^T, A, b) only, and $\max_{1 \leq i \leq (n-1)} |t_{i+1} - t_i| = O(n^{-1})$. Then for all n sufficiently large, the level set $\mathcal{S}_{z^*}$ is bounded for any $y \in \mathbb{R}^n$ and $z^* \in \mathbb{R}^\ell$.

Next we show that under the similar order condition on α, a directional vector d can always be found for the equation $H_{y,n}(z) + H'_{y,n}(z; d) = 0$ for any $z \in \mathbb{R}^\ell$. This result, along with boundedness of $\mathcal{S}_{z^*}$, ensures the global convergence of Algorithm 1 [8, Theorem 4].

Proposition 4.2: Suppose $\limsup_{n\to\infty} n\alpha^{-1} < 4\rho^{-1}$ and $\max_{1 \leq i \leq (n-1)} |t_{i+1} - t_i| = O(n^{-1})$. Then for all n sufficiently large, any $y \in \mathbb{R}^n$ and $z \in \mathbb{R}^\ell$, there exists a unique $d \in \mathbb{R}^\ell$ such that $H_{y,n}(z) + H'_{y,n}(z; d) = 0$.

Let $\{z^k\}$ be the sequence generated by Algorithm 1 from an initial vector z^0. Under the assumptions in Propositions 4.1 and 4.2, it follows from [8, Theorem 4] that if $\liminf \beta^{m_k} > 0$, then a limiting point of $\{z^k\}$ is a desired solution to the B-differentiable equation $H_{y,n}(z) = 0$.

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