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Interpolation and Approximation by Monotone Cubic Splines

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We study the reconstruction of a function defined on the real line from given, possibly noisy, data values and given shape constraints. Based on two abstract minimization problems characterization results are given for interpolation and approximation (in the euclidean norm) under monotonicity constraints. We derive from these results Newton-type algorithms for the computation of the monotone spline approximant.

1. INTRODUCTION

We consider the problem of reconstructing a real valued function, defined on an interval of the real line, from a finite sample of, possibly noisy, function values. We assume given a priori information about the shape of the function. The shape constraints restrict the reconstruction to some closed convex subset of the relevant function space. The approximation procedures used here include interpolation and least squares approximation. There may also be additional linear constraints; e.g., the sum of the fitted values should be equal to a given value. Our approach is based on using a minimization principle: the smoothing spline principle [25, 23]. This paper parallels our papers [2, 1, 11], in which we considered constraining the second derivative. For a similar approach see also [20, 17]. The starting point is a characterization of (a derivative of) the constrained smoothing spline as the orthogonal projection of a finite sum (with unknown coefficients) of certain basis functions. The projection is onto the convex set determined by the particular shape constraint at hand. The unknown coefficients are defined from interpolation conditions which lead to a set of nonlinear equations. These are solved by Newton's method.

The area of interpolation under monotonicity constraints has attracted considerable attention (the case of smoothing less). Early papers include

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[4, 19]. In [13] conditions on the derivatives are given to insure monotonicity of a piecewise C^1-cubic. This result was recently generalized in [8]. Other papers are [16, 26, 7, 9, 24] and more recently [3, 12]. The last paper also gives a nice overview of the area. Utreras in [27] studies approximation properties of monotone smoothing splines; see also (for interpolation) [3, 9].

To our knowledge Hornung [14] was the first to consider using a minimal principle when computing monotone interpolation splines. Dauner and Reinsch [5] have recently given algorithms for computing monotone (and positive; see also [22]) splines based on the minimization principle. Hornung [15] and Varas [28] use methods from optimal control to devise numerical methods. One difference between [5] and this paper is that, apart from the fact that in [5] only interpolation is considered, the algorithms in [5] are not of Newton type (they do not exhibit a quadratic rate of convergence). On the other hand the numerical results presented show that the suggested schemes perform quite well.

Our paper is organized as follows. In Section 2 we provide a self-contained proof of an important characterization theorem for constrained spline interpolation given by Micchelli and Utreras [21]. As a corollary a similar theorem for smoothing is obtained. Section 3 deals with monotonicity constraints. We apply the results of Section 2 and arrive at characterization results for interpolation, Theorem 3.4 (fixed end derivatives) and Theorem 3.9 (free end derivatives). Theorems 3.5 and 3.10 give the corresponding results for smoothing.

In order to transform the results of Section 3 into numerical algorithms, it is necessary to compute the orthogonal projections. In Section 4 we investigate the general structure of the projection operator for the case of monotonicity constraints. For the important case when the function to be projected is piecewise linear and continuous we provide the characterizations of the projection in Theorem 4.6. For this case we supply an algorithm which requires order n^2 operations ($n+2$ being the number of data points) for the computation of the projection.

In Section 5 Newton-type methods are derived, both for interpolation and for smoothing. We also give local convergence results for these schemes. In the last section we discuss computer implementation and present some numerical results.

2. Theory: General Convex Constraints

In this section we study two abstract convex minimization problems in a Hilbert space $\mathbf{H}$. The first, $\mathbf{P}_i$, corresponds to an interpolation problem and the second, $\mathbf{P}_a$, to an approximation problem.

$$\mathbf{P_i}: \text{ Minimize } \|f\|^2 \text{ when}$$

$$If = w \text{ and } f \in C \subset \mathbf{H} \tag{2.1}$$

$$\mathbf{P_a}: \text{ Minimize } p\,\|f\|^2 + (z-y)^{\mathrm{T}}\,Q(z-y) \text{ when}$$

$$If = Kz + u,\ Az = d, \text{ and } f \in C \subset \mathbf{H}. \tag{2.2}$$

Here C is a closed convex subset of $\mathbf{H}$ and $I: \mathbf{H} \to \mathbf{R}^n$ denotes a bounded linear mapping, I^* denotes its dual, and A, K are linear mappings. $K: \mathbf{R}^{n+l} \to \mathbf{R}^n$ has a full rank matrix, and $A: \mathbf{R}^{n+l} \to \mathbf{R}^m$. The vectors u, $w \in \mathbf{R}^n$, $y \in \mathbf{R}^{n+l}$, and $d \in \mathbf{R}^m$ are given, as well as the positive definite correlation matrix Q and the smoothing parameter $p > 0$. We may always, by the Riesz representation theorem, write

$$If = ((M_1, f), ..., (M_n, f))^{\mathrm{T}} = (M, f) \in \mathbf{R}^n, \tag{2.3}$$

where $M_i \in \mathbf{H}$, $i = 1, 2, ..., n$, and $M = (M_1, M_2, ..., M_n)^{\mathrm{T}} \in \mathbf{H}^n$. If $\alpha = (\alpha_1, \alpha_2, ..., \alpha_n)^{\mathrm{T}} \in \mathbf{R}^n$ we will use in the following the notation $\alpha^{\mathrm{T}} M = M^{\mathrm{T}} \alpha = \sum_{j=1}^n \alpha_j M_j$.

A theorem very similar to the following for $\mathbf{P_i}$ is given in [21]. We provide a self-contained proof.

THEOREM 2.1. *Suppose that* $\operatorname{int}(C) \cap I^{-1}(w) \neq \emptyset$. *Then* $\mathbf{P_i}$ *has a unique solution f and f has the structure*

$$f = P_C(\alpha^{\mathrm{T}} M) = P_C(I^* \alpha)$$

with P_C *denoting the projection onto the closed convex set* $C \subset \mathbf{H}$ *and* $\alpha = (\alpha_1, \alpha_2, ..., \alpha_n)^{\mathrm{T}}$ *some vector in* $\mathbf{R}^n$. *Conversely, if for* $\alpha \in \mathbf{R}^n$ *the vector* $f = P_C(\alpha^{\mathrm{T}} M)$ *satisfies the condition* $If = w$, *then f is the solution of* $\mathbf{P_i}$.

Proof. Since the domain of the mapping $f \mapsto \|f\|^2$ is the closed convex set $C \cap I^{-1}(w)$, it is clear that $\mathbf{P_i}$ has a unique solution which we denote by f and we may write

$$I^{-1}(w) = f + \{M_1, M_2, ..., M_n\}^{\perp}.$$

Let $\sum_{j=1}^n \beta_j M_i$ be the vector in $I^{-1}(w)$ having the smallest norm and $q = \sum_{j=1}^n \beta_j M_j - f$. Now take $C_1 = \{v \in I^{-1}(w) : (q, v - f) > 0\}$. We have that C_1 and C are convex, $f \in \partial C$, $\operatorname{int}(C) \neq \emptyset$, and $C \cap C_1 = \emptyset$; cf. Fig. 1. It is then a well-known consequence of the Hahn–Banach theorem (see, e.g., [18]) that there exists a hyperplane $\mathscr{P}$ through f with the equation $(n_f, v - f) = 0$, separating C and C_1 and so that $(n_f, v - f) < 0$ if $v \in \operatorname{int}(C)$ (n_f is an outward normal to C). Now there exists a vector $u_0 \in I^{-1}(w) \cap \operatorname{int}(C)$. Therefore $u_0 - f \in \{M_1, M_2, ..., M_n\}^{\perp}$ and $(n_f, u_0 - f) < 0$. It follows

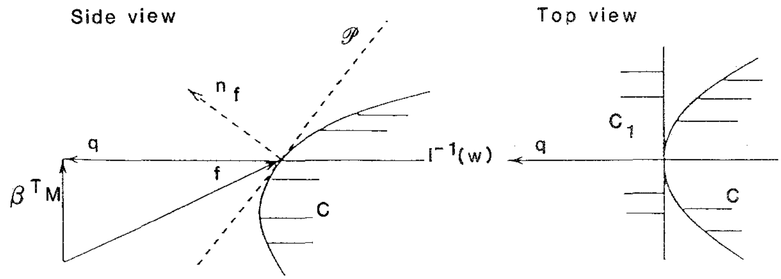

FIGURE 1

that the projection of n_f on $\{M_1, M_2, ..., M_n\}^{\perp}$ is non-vanishing. Since, by construction, $\mathscr{P} \cap I^{-1}(w) = \partial C_1$ it follows that this projection is a multiple of q. Since also $(q, u_0 - f) < 0$, this multiple is positive and therefore we may take

$$n_f = q + \sum_{i=1}^{n} \gamma_i M_i.$$

Now $f = P_C(f + n_f)$, where

$$f + n_f = \sum_{j=1}^{n} \beta_j M_j - q + q + \sum_{j=1}^{n} \gamma_j M_j = \sum_{j=1}^{n} \alpha_j M_j,$$

and therefore $f = P_C(\alpha^T M)$. By definition of duality,

$$\alpha^T(If) = ((I^*\alpha), f)_{\mathbf{H}},$$

whence we conclude, also using (2.3), that $I^*\alpha = \alpha^T M \in \mathbf{H}$.

Next assume that $\alpha \in \mathbf{R}^n$ is given and that $g = P_C(\alpha^T M)$ satisfies the condition $Ig = w$. Let $\beta'^T M$ denote the orthogonal projection of $\alpha^T M$ on $I^{-1}(w)$. It follows that $g = \beta'^T M - q'$, where q' is a normal vector to the set $I^{-1}(w) \cap C$. But $\beta'^T M$ must also be the projection of the null vector on $I^{-1}(w)$, previously denoted by $\beta^T M$. From this we conclude that $q' = q$ and that $g = f$. ▮

COROLLARY 2.2. *Suppose that*

$$\operatorname{int}(C) \cap \{f : \exists z, Az = d, If = Kz + u\} \neq \emptyset. \tag{2.4}$$

Then problem $\mathbf{P_a}$ *has a unique solution* $(f, z)^T \in \mathbf{H} \times \mathbf{R}^{n+l}$ *and this solution has the structure*

$$f = P_C(\alpha^T M) = P_C(I^*\alpha), \qquad z = y + pQ^{-1}(A^T\beta - K^T\alpha), \tag{2.5}$$

where $\alpha = (\alpha_1, \alpha_2, ..., \alpha_n)^{\mathrm{T}} \in \mathbf{R}^n$, $\beta = (\beta_1, \beta_2, ..., \beta_m)^{\mathrm{T}} \in \mathbf{R}^m$, *and* $M = (M_1, M_2, ..., M_n)^{\mathrm{T}} \in \mathbf{H}^n$. *Conversely, if* α *and* β *are given and if* f *and* z *as defined by* (2.5) *satisfy the side conditions in* (2.2), *then* $(f, z)^{\mathrm{T}}$ *is the solution of* $\mathbf{P_a}$.

Proof. Introduce the notation $F = \binom{f}{z}$ for elements in the Hilbert space $\mathbf{H} \times \mathbf{R}^{n+1} = \mathscr{H}$ with the inner product $\langle \cdot, \cdot \rangle$ defined by

$$\langle F_1, F_2 \rangle = (f_1, f_2)_{\mathbf{H}} + p^{-1} z_1^{\mathrm{T}} Q z_2.$$

Let $F_0 = \binom{0}{y}$. Also let $J\colon \mathscr{H} \to \mathbf{R}^n \times \mathbf{R}^m$ be defined by

$$J(F) = \begin{pmatrix} If - Kz \\ Az \end{pmatrix},$$

where $If = (M, f) \in \mathbf{R}^n$. We are to minimize $\| F - F_0 \|_{\mathscr{H}}^2$ when F is confined to the closed convex subset $C \times \mathbf{R}^{n+l} \in \mathscr{H}$ and satisfies the equation $J(F) = \binom{u}{d}$. Now the condition $\operatorname{int}(C \times \mathbf{R}^{n+l}) \cap J^{-1} \binom{u}{d} \neq \varnothing$ is equivalent to

$$\operatorname{int}(C) \times \mathbf{R}^{n+l} \cap \left\{ \begin{pmatrix} f \\ z \end{pmatrix} : If = Kz + u,\ Az = d \right\} \neq \varnothing,$$

i.e., to (2.4). According to the previous theorem we therefore have

$$F - F_0 = P_{(C \times \mathbf{R}^{n+l} - F_0)} \left(J^* \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \right) \tag{2.6}$$

for some element $(\alpha, \beta)^{\mathrm{T}} \in \mathbf{R}^n \times \mathbf{R}^m$, i.e.,

$$\begin{pmatrix} f \\ z \end{pmatrix} - \begin{pmatrix} 0 \\ y \end{pmatrix} = P_{(C \times \mathbf{R}^{n+l} - F_0)} \left(J^* \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \right).$$

To complete the proof we need to calculate $J^* \binom{\alpha}{\beta}$ when $\alpha \in \mathbf{R}^n$ and $\beta \in \mathbf{R}^m$. Suppose that $J^* \binom{\alpha}{\beta} = \binom{g}{c} \in \mathscr{H}$. Then, by duality,

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}^{\mathrm{T}} J(F) = \left\langle J^* \begin{pmatrix} \alpha \\ \beta \end{pmatrix}, F \right\rangle_{\mathscr{H}},$$

i.e.,

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} (M, f) - Kz \\ Az \end{pmatrix} = (g, f) + p^{-1} c^{\mathrm{T}} Q z,$$

i.e.,

$$(\alpha^{\mathrm{T}} M, f) - \alpha^{\mathrm{T}} K z + \beta^{\mathrm{T}} A z = (g, f) + p^{-1} c^{\mathrm{T}} Q z.$$

This is to be valid for all $f \in \mathbf{H}$ and $z \in \mathbf{R}^{n+l}$. Therefore

$$g = \alpha^{\mathrm{T}} M \in \mathbf{H} \qquad \text{and} \qquad c = pQ^{-1}(A^{\mathrm{T}}\beta - K^{\mathrm{T}}\alpha).$$

Finally, using that $F_0 = \binom{0}{y}$, we easily obtain

$$\begin{pmatrix} f \\ z \end{pmatrix} - \begin{pmatrix} 0 \\ y \end{pmatrix} = P_{(C \times \mathbf{R}^{n+l} - F_0)} \begin{pmatrix} g \\ c \end{pmatrix} = \begin{pmatrix} P_C(g) \\ c \end{pmatrix} \tag{2.7}$$

and it follows that $(f, z)^{\mathrm{T}}$ solves $\mathbf{P_a}$.

Conversely, if $(f, z)^{\mathrm{T}}$, as defined by (2.5), satisfies (2.7) it follows that $F = (f, z)^{\mathrm{T}}$ satisfies (2.6) and by the previous theorem F is the solution of $\mathbf{P_a}$. ∎

Remark 2.3. If, in particular, $A = 0$ and $d = 0$, i.e., if the condition $Az = d$ is not present, then, since K has full rank, the condition (2.4) is satisfied as soon as int $(C) \neq \varnothing$.

3. Theory: Monotonicity Constraints

In this section we apply the previous theory to problems $\mathbf{P_i}$ and $\mathbf{P_a}$ with a constraint set obtained by restricting the values of $x'(t)$, for example by requiring that $x'(t) \geqslant 0$ everywhere or that $\varphi(t) \leqslant x'(t) \leqslant \psi(t)$. In the analysis we make a difference between two cases. In the first case we assume that the derivative x' is given in one or both of the endpoints. In the second case we consider problems with free end derivatives, i.e., we impose no additional restrictions in the endpoints. Before proceeding let us recall the following characterization of projections in a Hilbert space, to be used later on. For a reference, see, for example, [18].

Remark 3.1. If $\mathbf{H}$ is a Hilbert space, $C \subset \mathbf{H}$ a closed convex subset, $u \in \mathbf{H}$, and $v \in C$ then $v = P_C(u)$ if and only if $(u - v, q)_{\mathbf{H}} \leqslant 0$ whenever $v + q \in C$.

We introduce some further notation. Let $\{(t_i, y_i)\}_{i=1}^{n+2}$, $a = t_1 < t_2 < \cdots < t_{n+2} = b$, be given data points in R^2 which are to be interpolated or approximated by some function $x(t)$, $t \in [a, b]$. Δ_i^1 and Δ_i^2 are first and second order divided differences of this data set,

$$\Delta_i^1 = \frac{y_{i+1} - y_i}{t_{i+1} - t_i}, \qquad \Delta_i^2 = \frac{\Delta_{i+1}^1 - \Delta_i^1}{t_{i+2} - t_i}.$$

The functions $M_i(t)$, $i = 1, 2, \ldots, n$, are now linear B-splines, i.e., functions which are continuous, are piecewise linear, have supp $M_i = [t_i, t_{i+2}]$, and are normalized so that $\int_a^b M_i(t)\,dt = \frac{1}{2}$. Similarly

$$M_0(t) = (t_2 - t)_+/(t_2 - t_1)^2 \quad \text{and} \quad M_{n+1}(t) = (t - t_{n+1})_+/(t_{n+2} - t_{n+1})^2$$

so that $\int_a^b M_0(t)\,dt = \int_a^b M_{n+1}(t)\,dt = \frac{1}{2}$. If $x(t)$ interpolates $\{(t_i, y_i)\}_{i=1}^{n+2}$ then Δ_0^2 and Δ_{n+1}^2 are defined as

$$\Delta_0^2 = (\Delta_1^1 - x'(a))/(t_2 - t_1) \quad \text{and} \quad \Delta_{n+1}^2 = (x'(b) - \Delta_{n+1}^1)/(t_{n+2} - t_{n+1})$$

and are naturally interpreted as second order divided differences with two coinciding knots $t_0 = t_1$ and $t_{n+2} = t_{n+3}$. The data vector is $y = (y_1, y_2, ..., y_{n+2})^{\mathrm{T}} \in \mathbf{R}^{n+2}$ and $z = (x(t_1), x(t_2), ..., x(t_{n+2}))^{\mathrm{T}}$ is the vector of function values, sometimes coinciding with y. By $W^2(a, b)$ we denote the Sobolev space of all functions x such that x' is absolutely continuous on (a, b) and $x'' \in L^2(a, b)$. Further let

$$C_a = \{x \in W^2(a, b) : x'(a) = x'_a\}, \tag{3.1}$$

$$C_{ab} = \{x \in W^2(a, b) : x'(a) = x'_a, \text{ and } x'(b) = x'_b\}, \tag{3.2}$$

where x'_a and x'_b are given constants.

Now let us consider the following constrained interpolation problem.

$$\mathbf{P_{i,m}(C')}\text{: Minimize} \int_a^b x''^2(t)\,dt \text{ when } x(t_i) = y_i,$$

$$i = 1, 2, ..., n+2, \text{ and } x \in \bar{C}_m \cap C',$$

$$\bar{C}_m = \{x \in W^2(a, b) : \varphi(t) \leqslant x'(t) \leqslant \psi(t)\}. \tag{3.3}$$

Here $C' = C_a$ or C_{ab} for the case with fixed end derivatives and $C' = W^2(a, b)$ for the case with free end derivatives. The bounds φ and ψ are measurable functions. We are primarily interested in the case when, e.g., $\varphi \equiv 0$, $\psi \equiv \infty$ or when φ and ψ are piecewise constant or linear. It is almost obvious that this problem has a unique solution, provided that $\bar{C}_m \cap C'$ contains at least one function x with $x(t_i) = y_i$ for $i = 1, 2, ..., n+2$. Similarly, consider the approximation problem

$$\mathbf{P_{a,m}(C')}\text{: Minimize } p \int_a^b x''^2(t)\,dt + (z - y)^{\mathrm{T}} Q(z - y) \text{ when } Az = d$$

$$\text{and } x \in \bar{C}_m \cap C',\ x(t_i) = z_i,\ i = 1, 2, ..., n+2.$$

Here Q is a positive definite matrix representing the correlation between stochastic errors in the data vector y and $p > 0$ is a smoothing parameter. The equation $Az = d$ with A an $m \times (n+2)$-matrix, $m < n+2$, imposes m

linear constraints on the vector $z=(x(t_1), x(t_2), ..., x(t_{n+2}))^{\mathrm{T}}$. If, e.g., the mean value of the function values is to be fixed, one should take $A=(1, 1, ..., 1)$. This problem also has a unique solution, provided that there exists at least one function $x \in \bar{C}_m \cap C'$ so that $Az=d$. In the following we will often refer to the problems $\mathbf{P}_{\mathrm{i,m}}(\mathbf{C}')$, $\mathbf{P}_{\mathrm{a,m}}(\mathbf{C}')$ as simply $\mathbf{P}_{\mathrm{i,m}}$, $\mathbf{P}_{\mathrm{a,m}}$, respectively. It should then be clear from the context which set C' is presumed.

We will make a reformulation of the problems $\mathbf{P}_{\mathrm{i,m}}$ and $\mathbf{P}_{\mathrm{a,m}}$ so as to conform to the abstract problems $\mathbf{P}_{\mathrm{i}}$ and $\mathbf{P}_{\mathrm{a}}$ of section 2. Taking divided second differences in Taylor's formula, one may easily establish the Peano formula (see [6]),

$$\int_a^b x''(t)\, M_i(t)\, dt = \Delta_i^2, \qquad i=1, 2, ..., n. \tag{3.4}$$

Moreover, if a function $f \in L^2(a, b)$ satisfies the condition

$$\int_a^b f(t)\, M_i(t)\, dt = \Delta_i^2, \qquad i=1, 2, ..., n, \tag{3.5}$$

then there is a unique function $x \in W^2(a, b)$ with $x(t_i)=y_i$ for $i=1, 2, ..., n+2$ and $x''=f$.

At this point it will be convenient to distinguish between the two cases, fixed and free end derivatives.

3A. *Fixed End Derivatives*

Here we consider problems $\mathbf{P}_{\mathrm{i,m}}(\mathbf{C}')$ and $\mathbf{P}_{\mathrm{a,m}}(\mathbf{C}')$ with $C'=C_a$ or C_{ab}; i.e., we require that the derivative x' be given in one endpoint or in both endpoints.

We now show that the monotonicity problems $\mathbf{P}_{\mathrm{i,m}}(\mathbf{C}')$ and $\mathbf{P}_{\mathrm{a,m}}(\mathbf{C}')$ are instances of the abstract problems $\mathbf{P}_{\mathrm{i}}$ and $\mathbf{P}_{\mathrm{a}}$. The variants given after "or" below apply to the case when both $x'(a)$ and $x'(b)$ are given.

We take C as the convex closed set

$$C=C_{x'_a}=\left\{f \in L^2(a, b) : \varphi(t) \leqslant x'_a + \int_a^t f(s)\, ds \leqslant \psi(t)\right\}. \tag{3.6}$$

Taylor's formula at $t=a$ may be written

$$(x'', M_0)=\Delta_0^2$$

and we conclude the following. If $f \in L^2(a, b)$ is given then there exists a function $x \in W^2(a, b)$ with

$$x'(a)=x'_a, \qquad x(t_i)=y_i, \qquad i=1, 2, ..., n, \qquad x''=f$$

if and only if f satisfies (3.5) and

$$(f, M_0) = \Delta_0^2.$$

Moreover x is unique. Further, by Taylor's formula at $t = b$, it follows that we have $x'(b) = x'_b$ if and only if f in addition satisfies

$$(f, M_{n+1}) = \Delta_{n+1}^2.$$

Therefore let $I: L^2(a, b) \to \mathbf{R}^{n+1}$, or $I: L^2(a, b) \to \mathbf{R}^{n+2}$, be defined by

$$If = ((M_0, f), (M_1, f), ..., (M_n, f))^{\mathrm{T}} = (M, f)^{\mathrm{T}}$$

or

$$If = ((M_0, f), (M_1, f), ..., (M_{n+1}, f))^{\mathrm{T}} = (M, f)^{\mathrm{T}}.$$

We then have

$$If = (\Delta_0^2, \Delta_1^2, ..., \Delta_n^2)^{\mathrm{T}} = \Delta^2 = Ky + u = w$$

or (3.7a)

$$If = (\Delta_0^2, \Delta_1^2, ..., \Delta_{n+1}^2)^{\mathrm{T}} = \Delta^2 = Ky + u = w,$$

where

$$u = -\frac{x'_a}{(t_2 - t_1)} (1, 0, 0, ..., 0)^{\mathrm{T}}$$

or (3.7b)

$$u = -\frac{x'_a}{(t_2 - t_1)} (1, 0, 0, ..., 0)^{\mathrm{T}} + \frac{x'_b}{(t_{n+2} - t_{n+1})} (0, 0, ..., 1)^{\mathrm{T}}$$

and where $K: \mathbf{R}^{n+2} \to \mathbf{R}^{n+1}$ or $K: \mathbf{R}^{n+2} \to \mathbf{R}^{n+2}$ is a mapping with a full rank, three-banded upper triangular matrix depending only on $t_1, t_2, ..., t_{n+2}$.

For the condition $(\operatorname{int} C) \cap I^{-1}(Ky + u) \neq \varnothing$ of Theorem 2.1 we now have the following lemma.

LEMMA 3.2. *Assume that*

$$\psi(t) \leqslant \liminf_{\tau \to t} \psi(\tau), \qquad \varphi(t) \geqslant \limsup_{\tau \to t} \varphi(\tau), \qquad a \leqslant t \leqslant b, \tag{3.8}$$

$$\inf_{t \in (a, b)} (\psi(t) - \varphi(t)) > 0, \tag{3.9}$$

$$\varphi(a) < x'_a < \psi(a), \qquad \varphi(b) < x'_b < \psi(b), \tag{3.10}$$

$$\int_{t_i}^{t_{i+1}} \varphi(s)\, ds < y_{i+1} - y_i < \int_{t_i}^{t_{i+1}} \psi(s)\, ds, \qquad i = 1, 2, ..., n-1. \tag{3.11}$$

Then $\operatorname{int}(C_{x'_a}) \cap I^{-1}(Ky + u) \neq \varnothing$.

Proof. Consider the open point set

$$\{(s, t) \subset \mathbf{R}^2 : \varphi(t) < s < \psi(t),\ a < t < b\} = \Omega \subset \mathbf{R}^2.$$

It can be shown (the argument is omitted) that there exists a C^∞-function $s(t)$, $a \leqslant t \leqslant b$, such that

$$\begin{aligned} &(s(t), t) \in \Omega, \qquad a < t < b, \\ &s(a) = x'_a, \qquad s(b) = x'_b \\ &y_1 + \int_a^{t_i} s(\tau)\, d\tau = y_i \qquad \text{for} \quad i = 1, 2, ..., n+2. \end{aligned} \tag{3.12}$$

Take $f_0(t) = s'(t)$. Then we have $f_0 \in C_{x'_a}$. Further it is clear that f_0 is an interior point of $C_{x'_a}$. By the construction $If_0 = Ky + u$ and the proof is complete. ∎

For the condition (2.4) of Corollary 2.2 we have the next lemma.

LEMMA 3.3. *Assume that* (3.8)–(3.10) *of Lemma* 3.2 *are valid. Also assume that the equation* $Az = d$ *has a solution* $z \in \mathbf{R}^{n+2}$ *satisfying*

$$\int_{t_i}^{t_{i+1}} \varphi(s)\, ds < z_{i+1} - z_i < \int_{t_i}^{t_{i+1}} \psi(s)\, ds. \tag{3.13}$$

Then the condition (2.4) *is satisfied.*

The proof is similar to that of the previous lemma and is omitted.

Using Lemmas 3.2 and 3.3 and the preceding discussion we obtain the following theorems for $\mathbf{P}_{\mathbf{i,m}}$ and $\mathbf{P}_{\mathbf{a,m}}$.

THEOREM 3.4. *Suppose that* φ *and* ψ *satisfy* (3.8)–(3.11). *Let* $C = C_{x'_a}$. *Then the unique solution* $x \in W^2(a, b)$ *of* $\mathbf{P}_{\mathbf{i,m}}$ *has the property that* $x'' = P_C(\alpha^{\mathrm{T}} M)$ *for some* $\alpha \in \mathbf{R}^{n+1}$ *or* $\mathbf{R}^{n+2}$. *Conversely, if* $\alpha \in \mathbf{R}^{n+1}$ *or* $\mathbf{R}^{n+2}$ *satisfies the system*

$$\int_a^b M P_C(\alpha^{\mathrm{T}} M)\, dt = Ky + u. \tag{3.14}$$

Then $x'' = P_C(\alpha^{\mathrm{T}} M)$.

THEOREM 3.5. *Suppose that* φ *and* ψ *satisfy* (3.8)–(3.10) *and that the equation* $Az = d$ *has some solution* z *satisfying* (3.13). *Let* $C = C_{x'_a}$. *Then the* *unique solution* $x \in W^2(a, b)$ *of the approximation problem* $\mathbf{P}_{\mathbf{a,m}}$ *has the property*

$$\begin{aligned} x'' &= P_C(\alpha^{\mathrm{T}} M), \\ z &= y + pQ^{-1}(A^{\mathrm{T}}\beta - K^{\mathrm{T}}\alpha) \end{aligned} \tag{3.15}$$

for some vectors $\alpha \in \mathbf{R}^{n+1}$ *or* $\mathbf{R}^{n+2}$ *and* $\beta \in \mathbf{R}^m$. α *and* β *can be found by solving the system*

$$\begin{aligned} &\int_a^b MP_C(\alpha^{\mathrm{T}} M)\, dt = Kz + u \\ &Az = d. \end{aligned} \tag{3.16}$$

Conversely, if α, β *solves* (3.16) *then* $x'' = P_C(\alpha^{\mathrm{T}} M)$.

3B. *Free End Derivatives*

We now consider $\mathbf{P}_{\mathbf{i,m}}(\mathbf{C}')$ and $\mathbf{P}_{\mathbf{a,m}}(\mathbf{C}')$ without any restrictions on $x'(a)$ or $x'(b)$ ($C' = W^2(a, b)$), i.e., with the constraint set

$$\bar{C}_m = \{x \in W^2(a, b) : \varphi(t) \leqslant x'(t) \leqslant \psi(t)\}.$$

In order to handle this case we first introduce the closed convex set

$$C = \left\{ (f, x'_a)^{\mathrm{T}} \in L^2(a, b) \times \mathbf{R} : \varphi(t) \leqslant x'_a + \int_a^t f(s)\, ds \leqslant \psi(t) \right\},$$

the vector

$$u_0 = -(1/(t_2 - t_1))(1, 0, 0, ..., 0)^{\mathrm{T}},$$

and

$$M = (M_0, M_1, ..., M_n)^{\mathrm{T}}.$$

Then we formulate, for $r \geqslant 0$, the versions $\mathbf{P}_{\mathbf{i}}(\mathbf{r})$ and $\mathbf{P}_{\mathbf{a}}(\mathbf{r})$ of $\mathbf{P}_{\mathbf{i}}$ and $\mathbf{P}_{\mathbf{a}}$.

$\mathbf{P}_{\mathbf{i}}(\mathbf{r})$: Minimize $\int_a^b f^2(t)\, dt + r x_a'^2$ when

$(M, f) - x'_a u_0 = Ky \in \mathbf{R}^{n+1}$ and $(f, x'_a) \in C$

$\mathbf{P}_{\mathbf{a}}(\mathbf{r})$: Minimize $\int_a^b f^2(t)\, dt + r x_a'^2 + p^{-1}(z - y)^{\mathrm{T}} Q(z - y)$ when

$z \in \mathbf{R}^{n+2}$, $Az = d \in \mathbf{R}^m$, $(M, f) - x'_a u_0 = Kz \in \mathbf{R}^{n+1}$,

and $(f, x'_a)^{\mathrm{T}} \in C$.

Consider first the case when $r > 0$. Let $\mathbf{H} = L^2(a, b) \times \mathbf{R}$ have its norm defined by $\|(f, x'_a)^{\mathrm{T}}\|^2 = \int_a^b f^2(t)\, dt + r x'^2_a$ and let $I: \mathbf{H} \to \mathbf{R}^{n+1}$ be given by

$$I\begin{pmatrix} f \\ x'_a \end{pmatrix} = (M, f) - x'_a u_0.$$

It follows by Theorem 2.1 and Corollary 2.2 that the solutions $(f_r, x'_{ar})^{\mathrm{T}}$ are of the form

$$\begin{pmatrix} f_r \\ x'_{ar} \end{pmatrix} = P_C(I^*(\alpha))$$

for some $\alpha \in \mathbf{R}^{n+1}$. It is straightforward to verify that

$$I^*(\alpha) = \begin{pmatrix} \alpha^{\mathrm{T}} M \\ (1/r)\, \alpha^{\mathrm{T}} u_0 \end{pmatrix} = \begin{pmatrix} \alpha^{\mathrm{T}} M \\ \alpha_0/(r(t_2 - t_1)) \end{pmatrix}.$$

In order to apply Theorem 2.1 and Corollary 2.2 we need the following lemmas.

LEMMA 3.6. *Assume that* (3.8), (3.9), *and* (3.10) *are valid. Then* $\operatorname{int}(C) \cap I^{-1}(Ky) \neq \varnothing$.

Proof. Take the constants $x'_a \in (\varphi(a), \psi(a))$ and $x'_b \in (\varphi(b), \psi(b))$. Define the function $s(t)$ as in the proof of Lemma 3.2 and let $f(t) = s'(t)$. Then $(f, x'_a)^{\mathrm{T}}$ is an interior point of C. ∎

LEMMA 3.7. *Assume that* (3.8) *and* (3.9) *are valid and the equation* $Az = d$ *has at least one solution* z *satisfying* (3.13). *Then* $\operatorname{int}(C) \cap I^{-1}(Kz) \neq \varnothing$.

The proof is similar to the preceding proof and is omitted. By these lemmas and Theorem 2.1 and Corollary 2.2 we conclude that

$$\begin{pmatrix} f_r \\ x'_{ar} \end{pmatrix} = P_C \begin{pmatrix} \alpha^{\mathrm{T}} M \\ \alpha_0/(r(t_2 - t_1)) \end{pmatrix}. \tag{3.17}$$

Now, by Remark 3.1, (3.17) is equivalent to the condition that

$$\varphi(t) \leqslant x'_{ar} + \Delta x'_{ar} + \int_a^t (f_r + g)\, ds \leqslant \psi(t)$$

$$\Rightarrow \int_a^b (\alpha^{\mathrm{T}} M - f_r)\, g\, ds + r\left[\frac{\alpha_0}{r(t_2 - t_1)} - x'_{ar}\right] \Delta x'_{ar} \leqslant 0. \tag{3.18}$$

Suppose that $\varphi(a) < x'_{ar} < \psi(a)$. Then, for some $\varepsilon > 0$, we have for $t \in [a, a+\varepsilon)$

$$\varphi(t) < x'_{ar} + \Delta x'_{ar} + \int_a^t (f_r + g)\, ds < \psi(t)$$

whenever $\operatorname{supp} g \subset [a, a+\varepsilon)$ and g and $\Delta x'_{ar}$ are small enough. Take g with $\operatorname{supp} g \subset [a, a+\varepsilon)$ and $\Delta x'_{ar}$ so that $\Delta x'_{ar} + \int_a^b g\, ds = 0$. It follows that

$$\int_a^b (\alpha^{\mathrm{T}} M - f_r - \alpha_0/(t_2 - t_1) + r x'_{ar})\, g\, ds \leqslant 0$$

for all such g, whence we conclude that

$$\alpha^{\mathrm{T}} M - f_r - \alpha_0/(t_2 - t_1) + r x'_{ar} = 0 \qquad \text{for} \quad t \in [a, a+\varepsilon).$$

Taking $t = t_1$ we obtain

$$f_r(t_1) = r x'_{ar}. \tag{3.19}$$

Conversely, suppose that for some $x'_{ar} \in (\varphi(a), \psi(a))$ we have

$$f_r = P_{C_{x'_{ar}}}(\alpha^{\mathrm{T}} M),$$

where $C_{x'_{ar}} \subset L^2(a, b)$ is defined by (3.6), and that (3.19) holds. We claim that

$$\begin{pmatrix} f_r \\ x'_{ar} \end{pmatrix} = P_C \begin{pmatrix} \alpha^{\mathrm{T}} M \\ \alpha_0/(r(t_2 - t_1)) \end{pmatrix}.$$

To prove the claim we first note, using the implication

$$\varphi(t) \leqslant x'_{ar} + \int_a^t (f_r + g)\, ds \leqslant \psi(t) \Rightarrow \int_a^b (\alpha^{\mathrm{T}} M - f_r)\, g\, ds \leqslant 0,$$

that $\alpha^{\mathrm{T}} M - f_r$ is constant on some interval $[a, a+\varepsilon)$ and the constant is

$$\alpha^{\mathrm{T}} M(t_1) - f_r(t_1) = \frac{\alpha_0}{(t_2 - t_1)} - r x'_{ar}.$$

Therefore, if

$$\varphi(t) \leqslant x'_{ar} + \Delta x'_{ar} + \int_a^t (f_r + g)\, ds \leqslant \psi(t), \qquad \text{for} \quad t \in (a, b)$$

then we have

$$\int_a^b (\alpha^T M - f_r)\, g\, ds + \left[\frac{\alpha_0}{(t_2-t_1)} - r x'_{ar}\right] \Delta x'_{ar} = \int_a^b (\alpha^T M - f_r)\, g_1\, ds,$$

where g_1 is defined by

$$g_1 = \begin{cases} g(t) + \Delta x'_{ar}/\varepsilon & \text{for} \quad t \in [a, a+\varepsilon) \\ g(t) & \text{for} \quad t \in [a+\varepsilon, b) \end{cases}$$

Now

$$\begin{aligned} &x'_{ar} + \int_a^t (f_r + g_1)\, ds \\ &\quad = \begin{cases} x'_{ar} + (t-a)\, \Delta x'_{ar}/\varepsilon + \int_a^t g\, ds & \text{if} \quad t \in [a, a+\varepsilon) \\ x'_{ar} + \Delta x'_{ar} + \int_a^t g\, ds & \text{if} \quad t \in [a+\varepsilon, b). \end{cases} \end{aligned}$$

If ε is small enough we have

$$\varphi(t) \leqslant x'_{ar} + \int_a^t (f_r + g_1)\, ds \leqslant \psi(t), \qquad \text{for} \quad t \in (a, b)$$

and we conclude that

$$\begin{aligned} &\int_a^b (\alpha^T M - f_r)\, g_1\, ds \\ &\quad = \int_a^b (\alpha^T M - f_r)\, g\, ds + \left[\frac{\alpha_0}{t_2 - t_1} - r x'_{ar}\right] \Delta x'_{ar} \leqslant 0, \end{aligned}$$

which proves the claim.

To summarize we may now formulate the following theorem.

THEOREM 3.8. *Let $r > 0$ and assume, for the problem $\mathbf{P}_i(\mathbf{r})$, that φ and ψ satisfy* (3.8), (3.9), (3.11) *and for the problem $\mathbf{P}_a(\mathbf{r})$ that they satisfy* (3.8), (3.9) *and that equation $Az = d$ has some solution z satisfying* (3.13). *Then for the unique solution $(f_r, x'_{ar})^T$ of $\mathbf{P}_i(\mathbf{r})$ or $\mathbf{P}_a(\mathbf{r})$ we have*

$$f_r = P_{C_{x'_{ar}}}(\alpha^T M) \text{ for some } \alpha \in \mathbf{R}^{n+1} \text{ and } x'_{ar} \in [\varphi(a), \psi(a)].$$

Moreover

$$f_r(t_1) = r x'_{ar} \qquad \text{if} \quad \varphi(a) < x'_{ar} < \psi(a).$$

Conversely, if

$$f_r = P_{C_{x'_{ar}}}(\alpha^T M) \qquad \text{for some } \alpha \in \mathbf{R}^{n+1},$$

$f_r(t_1)=rx'_{ar}$, $\varphi(a)<x'_{ar}<\psi(a)$ and if, for the problem $\mathbf{P_i(r)}$,

$$\int_a^b f_r M\,dt = Ky + x'_{ar}u_0$$

and for the problem $\mathbf{P_a(r)}$,

$$\int_a^b f_r M\,dt = Kz + x'_{ar}u_0, \qquad z = y + pQ^{-1}(A^{\mathrm{T}}\beta - K^{\mathrm{T}}\alpha)$$

then f_r is the solution of $\mathbf{P_i(r)}$ *and* $\mathbf{P_a(r)}$, *respectively.*

Now let $h(r)$ denote the minimum value for $\mathbf{P_i(r)}$ and $\mathbf{P_a(r)}$. One can prove that $h(r)$ is continuous for $r \geqslant 0$ and that $\int_a^b f_r^2(s)\,ds$ and x'_{ar} are bounded. Therefore $h(0)=h(0_+)$ and for some subsequence of r-values tending to zero, we have

$$f_r \to f_0 \qquad \text{weakly in } L^2(a,b) \text{ and } x'_{ar} \to x'_{a0}.$$

Using that $\mathbf{P_i(0)}$ and $\mathbf{P_a(0)}$ have unique solutions and that the functional $f \mapsto \int_a^b f^2\,dt$ is uniformly convex, it follows that $f_r \to f_0$ strongly in $L^2(a,b)$ and that $x_{ar} \to 0$ as $r \to 0+$ through all real values. Therefore we have either $x'_{a0}=\varphi(a)$ or $\psi(a)$, or $f_0(t_1)=0$ and $\varphi(a)<x'_{a0}<\psi(a)$.

From the preceding we obtain the following theorems.

THEOREM 3.9. *Assume that φ and ψ satisfy* (3.8), (3.9), *and* (3.11). *Then problem* $\mathbf{P_{i,m}(C')}$ *with $C'=W^2(a,b)$ has a unique solution x, with the property that*

$$x'' = P_{C'_{x_a}}(\alpha^{\mathrm{T}}M), \qquad \text{where } x'(a)=x'_a \in [\varphi(a), \psi(a)] \text{ and } \alpha \in \mathbf{R}^{n+1}.$$

Further, we have either $\varphi(a)<x'_a<\psi(a)$ and $x''(t_1)=0$, or $x'_a=\varphi(a)$ or $\psi(a)$. Conversely, if α, x'_a solves the system

$$\begin{aligned} &\int_a^b MP_{Cx'_a}(\alpha^{\mathrm{T}}M)\,dt = Ky + x'_a u_0 \\ &f(t_1) = P_{Cx'_a}(\alpha^{\mathrm{T}}M)(t_1) = 0, \end{aligned} \tag{3.20}$$

where $\varphi(a)<x'_a<\psi(a)$ then $x''=P_{Cx'_a}(\alpha^{\mathrm{T}}M)$.

THEOREM 3.10. *Assume that φ and ψ satisfy* (3.8) *and* (3.9). *Also assume that the equation $Az=d$ has at least one solution satisfying* (3.13). *Then* $\mathbf{P_{a,m}(C')}$ *with $C'=W^2(a,b)$ has a unique solution x, with the property that*

$$x''=P_{C'_a}(\alpha^{\mathrm{T}}M), \qquad \text{where } x'(a)=x'_a \in [\varphi(a),\psi(a)] \text{ and } \alpha \in \mathbf{R}^{n+1},$$
$$z = y + pQ^{-1}(A^{\mathrm{T}}\beta - K^{\mathrm{T}}\alpha).$$

Further, we have either $\varphi(a) < x'_a < \psi(a)$ and $x''(t_1) = 0$, or $x'_a = \varphi(a)$ or $\psi(a)$. Conversely, if α, x'_a solves the system

$$\begin{aligned} &\int_a^b MP_{C_{x'_a}}(\alpha^{\mathrm{T}} M)\, dt = Kz + x'_a u_0 \\ &f(t_1) = P_{C_{x'_a}}(\alpha^{\mathrm{T}} M)(t_1) = 0 \qquad (3.21) \\ &Az = d, \end{aligned}$$

where $\varphi(a) < x'_a < \psi(a)$, then $x'' = P_{C_{x'_a}}(\alpha^{\mathrm{T}} M)$.

4. The Projection Operators

In this section we assume that $x'_a \in \mathbf{R}$ is given and that

$$C = C_{x'_a} = \left\{ f \in L^2(a, b) : \varphi(t) \leqslant x'_a + \int_a^t f(s)\, ds \leqslant \psi(t) \right\},$$

where x'_a, φ, and ψ satisfy (3.8)–(3.10). In the main part of the section we investigate the general structure of the projection $v = P_C(u)$, for an arbitrary $u \in L^2(a, b)$. Finally we use these properties to construct a numerical algorithm for computing $P_C(u)$ when u is piecewise linear and continuous.

Let us start by introducing some notation. E_+ and E_- are relatively open subsets of $[a, b]$, defined by

$$E_- = \left\{ t \in [a, b] : \varphi(t) < x'_a + \int_a^t v(s)\, ds \right\} \qquad (4.1)$$

$$E_+ = \left\{ t \in [a, b] : x'_a + \int_a^t v(s)\, ds < \psi(t) \right\}. \qquad (4.2)$$

Further let $E^c_\pm = (a, b) \backslash E_\pm$. It is clear that $[a, b] = E_+ \cup E_-$ and that $E_+ \cap E_- \neq \varnothing$.

THEOREM 4.1. *Assume that $v \in C$ and that $u \in L^2(a, b)$. Then $v = P_C(u)$ if and only if the following conditions are satisfied.*

$$(u - v)' \text{ is a finite measure on } (a, b), \qquad (4.3)$$

$$(u - v)' \leqslant 0 \quad \text{on} \quad E_- \cap (a, b), \qquad (4.4)$$

$$(u - v)' \geqslant 0 \quad \text{on} \quad E_+ \cap (a, b), \qquad (4.5)$$

$$(u - v)(b_-) \geqslant 0 \quad \text{if} \quad b \in E_-, \qquad (4.6)$$

$$(u - v)(b_-) \leqslant 0 \quad \text{if} \quad b \in E_+. \qquad (4.7)$$

Proof. Suppose first that $v = P_C(u)$. Take any $Q \in W^1(a, b)$ with $\operatorname{supp} Q \subset E_- \cap (a, b)$ and such that $Q \leqslant 0$. It follows that $v + \varepsilon Q' \in C$ if $\varepsilon > 0$ is small enough. Hence we conclude that $\int_a^b (u-v)(s)\, Q'(s)\, ds \leqslant 0$, i.e., that $(u-v)'|_{E_- \cap (a,b)}$ is a finite negative measure. Similarly it follows that $(u-v)'|_{E_+ \cap (a,b)}$ is a finite positive measure and we have proved (4.3)–(4.5). Next assume that $b \in E_-$. Then, if $\delta > 0$ is small enough, $[b-\delta, b] \subset E_-$. Therefore, taking

$$Q(s) = \begin{cases} (b-\delta-s)/\delta & \text{if } \; b-\delta < s \leqslant b \\ 0 & \text{otherwise,} \end{cases} \tag{4.8}$$

we have

$$\int_{(a,b)} (u-v)(s)\, Q'(s)\, ds = \frac{-1}{\delta} \int_{(b-\delta,\, b)} (u-v)(s)\, ds \leqslant 0, \tag{4.9}$$

i.e.,

$$\frac{1}{\delta} \int_{(b-\delta,\, b)} (u-v)(s)\, ds \geqslant 0. \tag{4.10}$$

Taking limits as $\delta \to 0_+$ we obtain (4.6). Condition (4.7) follows similarly.

Conversely, assume that $v \in C$ and that (4.3)–(4.7) are valid. We are to show that $v = P_C(u)$, i.e., that

$$\int_a^b (u-v)(s)\, q(s)\, ds \leqslant 0 \qquad \text{whenever } w = v + q \in C. \tag{4.11}$$

Therefore take $Q(t) = \int_a^t q(s)\, ds$ so that

$$\int_{(a,b)} (u-v)(s)\, q(s)\, ds$$

$$= (u-v)(b_-)\, Q(b) - \int_{(a,b)} Q(s)\, d(u-v)(s). \tag{4.12}$$

Now if $s \notin E_-$ then

$$Q(s) = \int_a^s (w(\tau) - v(\tau))\, d\tau = x'_a + \int_a^s w(\tau)\, d\tau - \left[x'_a + \int_a^s v(\tau)\, d\tau \right]$$

$$= x'_a + \int_a^s w(\tau)\, d\tau - \varphi(s) \geqslant 0.$$

Similarly, if $s \notin E_+$ then

$$Q(s) = x'_a + \int_a^s w(\tau)\,d\tau - \left[x'_a + \int_a^s v(\tau)\,d\tau\right]$$
$$= x'_a + \int_a^s w(\tau)\,d\tau - \psi(s) \leqslant 0.$$

If, finally, $s \in E_+ \cap E_- \cap (a, b)$ then $(u-v)' = 0$. For the last term in (4.12) we therefore obtain, using (4.4) and (4.5),

$$-\int_{(a,b)} Q(s)\,d(u-v)(s)$$
$$= -\int_{E_+ \cap E_- \cap (a,b)} Q(s)\,d(u-v)(s)$$
$$-\int_{E_-^c} Q(s)\,d(u-v)(s) - \int_{E_+^c} Q(s)\,d(u-v)(s) \leqslant 0. \qquad (4.13)$$

Consequently

$$\int_{(a,b)} (u-v)(s)\,q(s)\,ds \leqslant (u-v)(b_-)\,Q(b).$$

If $b \notin E_-$ then $Q(b) \geqslant 0$ and so by (4.7) we have $(u-v)(b_-) \leqslant 0$. If $b \notin E_+$ then $Q(b) \leqslant 0$ and by (4.6) we have $(u-v)(b_-) \geqslant 0$. Finally if $b \in E_- \cap E_+$ then by (4.6) and (4.7) $(u-v)(b_-) = 0$. Therefore (4.11) is true and the proof is complete. ∎

As a special case we have the following corollary.

COROLLARY 4.2. *If $\psi \equiv \infty$ then $(u-v)' \geqslant 0$ everywhere in (a, b) and $(u-v)' = 0$ on E_-. Moreover $(u-v)(b_-) \leqslant 0$ and $v \geqslant u$. Finally, if $x'_a + \int_a^b v(s)\,ds > \varphi(b)$ then $(u-v)(b_-) = 0$.*

In order to construct explicit algorithms for the computation of $P_C(u)$ it is convenient to extract additional information about $v = P_C(u)$ under various assumptions on the regularity of u, φ, and ψ. In the following $\varphi'_\pm(t_0)$ denotes the left and right derivatives at t_0, i.e.,

$$\varphi'_\pm(t_0) = \lim_{t \to t_0 \pm} (\varphi(t) - \varphi(t_0))/(t - t_0).$$

By $\mathrm{BV}(a, b) \subset L^2(a, b)$ we understand the class of functions with bounded variation.

THEOREM 4.3. *Assume that* $u \in \mathrm{BV}(a, b)$. *Then* $v = P_C(u) \in \mathrm{BV}(a, b)$. *Further, if* $t \in E_-^c$ *and if* $\varphi'_\pm(t)$ *exist then*

$$v(t_+) \geqslant \varphi'_+(t) \qquad \text{and} \qquad v(t_-) \leqslant \varphi'_-(t). \tag{4.14}$$

Moreover

$$\varphi'_+(t) - \varphi'_-(t) \leqslant u(t_+) - u(t_-). \tag{4.15}$$

Similarly, if $t \in E_+^c$ *and if* $\psi'_\pm(t)$ *exist then*

$$v(t_+) \leqslant \psi'_+(t) \qquad \text{and} \qquad v(t_-) \geqslant \psi'_-(t), \tag{4.16}$$

$$\psi'_+(t) - \psi'_-(t) \geqslant u(t_+) - u(t_-). \tag{4.17}$$

Proof. Let $t \in E_-^c$. Then we have $x'_a + \int_a^\tau v(s)\, ds \geqslant \varphi(\tau)$ with equality for $\tau = t$. Therefore $\int_t^\tau v(s)\, ds \geqslant \varphi(\tau) - \varphi(t)$, whence (4.14) follows. Since, by (4.5), $(u-v)' \geqslant 0$ in a neighbourhood of t we obtain

$$\varphi'_+(t) - \varphi'_-(t) \leqslant v(t_+) - v(t_-) \leqslant u(t_+) - u(t_-). \tag{4.18}$$

The inequalities (4.16) and (4.17) follow similarly. ∎

COROLLARY 4.4. *Suppose, in addition, that* φ *or* ψ *are differentiable at* t *and that* u *is continuous at* t. *Then* v *is continuous at* t *and* $v(t) = \varphi'(t)$ *or* $v(t) = \psi'(t)$, *respectively.*

Proof. By (4.18) we have $0 \leqslant v(t_+) - v(t_-) \leqslant 0$. ∎

The next theorem deals with a case which is important for applications.

THEOREM 4.5. *Assume that* u, φ, *and* ψ *are piecewise linear and continuous and that* $v = P_C(u)$. *Then* $E_+ \cap E_-$ *consists of at most finitely many disjoint open intervals. Moreover, on each such interval* $u - v$ *is constant.*

Proof. Suppose on the contrary that $E_+ \cap E_-$ is the union of infinitely many disjoint open intervals. Then the endpoints of these intervals must have an accumulation point t_0 belonging either to $[a, b] \setminus E_-$ or $[a, b] \setminus E_+$. Without loss of generality assume that $t_0 \in [a, b] \setminus E_-$ and that the intervals $I_k = (a_k, b_k) \subset E_- \cap E_+$ are located to the right of t_0 and that $a_k \to t_{0+}$ as $k \to \infty$. Now there exists an $\varepsilon > 0$ so that u and φ are linear on $(t_0, t_0 + \varepsilon)$ with $u'(t) = \alpha$ and $\varphi'(t) = \beta$ and we may assume that $(t_0, t_0 + \varepsilon) \supset \bigcup_{k=1}^\infty I_k$. If $\varepsilon > 0$ is small enough we also have $(t_0, t_0 + \varepsilon) \subset E_+ \cap (a, b)$ and by (4.4) and (4.5) we conclude that

$$(u - v)' = 0 \qquad \text{on} \quad \bigcup_{k=1}^{\infty} I_k \subset (t_0, t_0 + \varepsilon) \tag{4.19}$$

$$(u - v)' \geqslant 0 \qquad \text{on} \quad (t_0, t_0 + \varepsilon). \tag{4.20}$$

By (4.19), $v(t)=u(t)+c_k$ if $t \in I_k$. By Corollary 4.4 it follows that

$$v(a_k)=v(b_k)=\varphi'(a_k)=\varphi'(b_k)=\beta \qquad \text{for all } k. \tag{4.21}$$

Therefore

$$u(t)=\beta-c_k \qquad \text{if} \quad t \in I_k$$

and since u is linear on $(t_0, t_0+\varepsilon) \supset \bigcup_{k=0}^{\infty}$ we conclude that $u(t)$ is constant on $(t_0, t_0+\varepsilon)$. But then $u'=0$ and by (4.19) and (4.20) we conclude that

$$v'=0 \qquad \text{on} \quad \bigcup_{k=1}^{\infty} I_k \subset (t_0, t_0+\varepsilon) \tag{4.22}$$

$$v' \leqslant 0 \qquad \text{on} \quad (t_0, t_0+\varepsilon). \tag{4.23}$$

Equations (4.22) and (4.21) then imply that

$$v(t)=\beta \qquad \text{on} \quad \bigcup_{k=1}^{\infty} I_k \subset (t_0, t_0+\varepsilon) \tag{4.24}$$

$$v'(t) \leqslant 0 \qquad \text{on} \quad (t_0, t_0+\varepsilon), \tag{4.25}$$

which actually implies that $v(t)=\beta=\varphi'(t)$ on $(t_0, t_0+\varepsilon)$, i.e., that $(t_0, t_0+\varepsilon) \subset [a, b] \backslash E_-$. This is a contradiction and consequently the number of intervals I_k is finite. By (4.4) and (4.5) we have $(u-v)'=0$ on each I_k, whence the last statement of the theorem follows. ▌

With the notation of Section 3 we now make a few observations about the case when $u=\alpha^{\mathrm{T}} M$ and when φ and ψ are also piecewise linear continuous functions, possibly over a different set of intervals. Consider, for example, the set $[a, b] \backslash E_- = \{t : x_a' + \int_a^t v(s)\, ds = \varphi(t)\}$. This set consists, by Theorem 4.5, of at most finitely many disjoint closed sets $J_i=[b_i, a_{i+1}]$ and we have the following possibilities.

(i) J_i does not contain any point where φ' has a jump discontinuity. By Corollary 4.4, $v(t)=\varphi'(t)$ is constant on J_i. Moreover, v is continuous at the endpoints of J_i.

(ii) If J_i contains some point t_0 where φ' has a jump discontinuity, then v may have a jump discontinuity at t_0 satisfying (4.14) and, by (4.18),

$$\varphi'_+(t_0)-\varphi'_-(t_0) \leqslant v(t_{0+})-v(t_{0-}) \leqslant 0. \tag{4.26}$$

A necessary condition for this possibility is that $\varphi'_+(t_0) \leqslant \varphi'_-(t_0)$. Similar statements are of course true for the set $[a, b] \backslash E_+$. We conclude that the projection $v=P_C(u)$ is continuous and piecewise linear if φ and ψ are piecewise linear and continuous and if

$$\varphi'_+ \geqslant \varphi'_-, \qquad \psi'_+ \leqslant \psi'_- \tag{4.27}$$

everywhere (i.e., case (ii) cannot appear). The solution x of problem $\mathbf{P}_{\mathbf{i,m}}$ or problem $\mathbf{P}_{\mathbf{a,m}}$ in this case is consequently a cubic spline, which is C^2-continuous.

We finish this section by indicating very briefly an algorithm for the numerical computation of $v = P_C(u)$ for the case when x'_a is fixed, $u = \alpha^T M$, $\psi \equiv \infty$, and $\varphi(t)$ is linear on the whole of $[a, b]$. To this end we formulate a theorem which summarizes the previous discussion and Corollary 4.2.

THEOREM 4.6. *Let $C = C_{x'_a}$ be defined by* (3.6), *where x'_a is given, $\varphi(t)$ is linear on (a, b), and $\psi(t) \equiv \infty$. Assume that u is piecewise linear and continuous. Then for the projection $v = P_C(u)$ it holds that*

(i) *$v(t) \geqslant u(t)$ on (a, b).*

(ii) *v is continuous and $(u - v)' \geqslant 0$ everywhere.*

(iii) *$v(t) = u(t) + c_i$ on $I_i = (a_i, b_i) \subset (a, b)$, $i = 1, 2, ..., L$, $a_i < b_i \leqslant a_{i+1}$, $c_i > c_{i+1} \geqslant 0$.*

(iv) *$v(t) = \varphi'(t)$ outside $\bigcup_{i=1}^{L} I_i$.*

(v) *On each interval I_i it holds that*

$$x'_a + \int_a^t v(s)\, ds > \varphi(t).$$

Since $x'_a + \int_a^t v(s)\, ds - \varphi(t)$ is a function which is a piecewise second degree polynomial over the intervals (t_i, t_{i+1}), $i = 1, 2, ..., n+1$, the following algorithm requires, apart from rational and logical operations, only that we solve equations of the first or second degree on the intervals (t_i, t_{i+1}). Apart from round-off errors the algorithm is exact. The maximal number of operations needed is $O(n^2)$.

Algorithm for Computing the Projection $v = P_C(u)$ of Theorem 4.6

1. $k := 1, \bar{t} := a.$
2. $c := \min\{c : x'_a + \int_a^t [u(s) + c]\, ds - \varphi(t) \geqslant 0, a \leqslant t \leqslant b\}.$
3. **If** $c \leqslant 0$ **then** $v = u$. **Go to end.**
4. $h(t) := x'_a + \int_a^t [u(s) + c]\, ds - \varphi(t).$
5. **If** $\bar{t} < b$ **then**

$$t^* := \min\{t : t \in [\bar{t}, b], h(t) = 0\},$$

$$t^{**} := \max\{t : t \in [\bar{t}, b], h(t) = 0\},$$

else go to end.

6. **If** $t^* < t^{**}$ **then**

$$a_k := t^*, b_k := t^{**}, c_k := c, k := k + 1.$$

7. **If** $t^* = t^{**} = b$, **then**

$$a_k := \bar{t},\ b_k := t^*,\ c_k := c.$$

Go to end.

8. $\bar{t} := t^{**}$.
9. **If** $\bar{t} = b$, **then go to end.**
10. $T := \sup\{t : t \in (\bar{t}, b],\ h'(t) > 0\}$.
11. $\tau := \max\{\tau : \tau \in (\bar{t}, T),\ \int_\tau^t [u(s) - u(\tau)]\, ds \geqslant 0,\ \tau < t \leqslant b\}$
12. $c := c - u(\tau)$, $h := h - h(\tau)$, $u := u - u(\tau)$, $\bar{t} := \tau$.
13. **Go to** 5.

End.

Figure 2a illustrates the geometrical construction of $P_C(\alpha^T M)$ for the case $\varphi = 0$, $\psi = \infty$, and $x'_a = 0$. Figure 2c shows a case when $\varphi = 0 < \psi =$

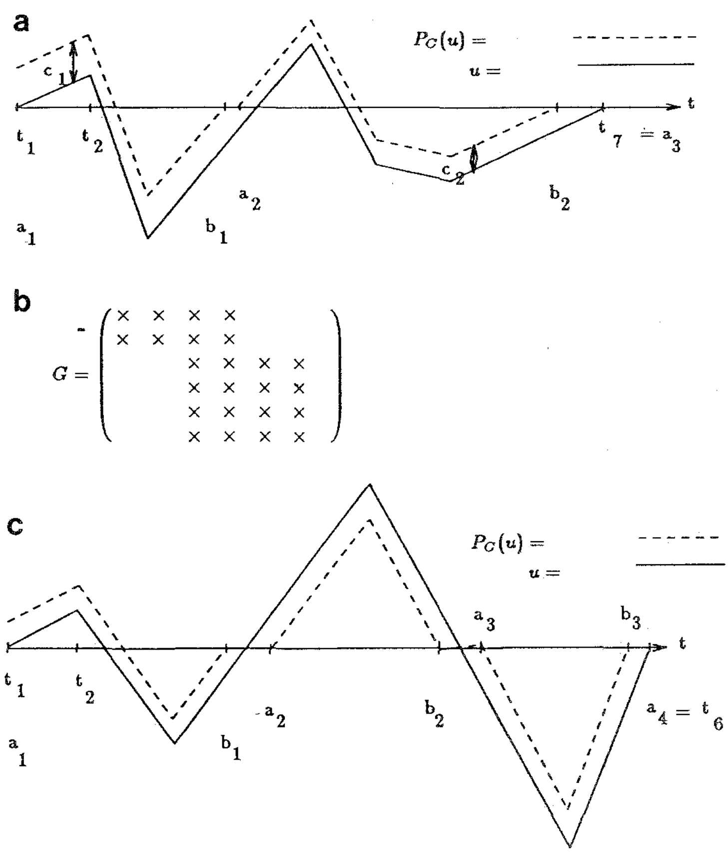

FIG. 2. (a) $P_C(u)$, when $x'(a) = 0$, $\varphi = 0$, and $\psi = \infty$. (b) Structure of matrix G for the example in (a). (c) $P_C(u)$, when $x'(a) = 0$, $\varphi = 0$, and $\psi = \text{constant} < \infty$.

constant and $x'_a = 0$ (this last case however is not covered in the algorithm above). We remark that it would be interesting to generalize the algorithm to include both upper and lower constraints.

5. Algorithms

In this section we provide Newton-type methods for problems $\mathbf{P}_{\mathbf{i},\mathbf{m}}(\mathbf{C}')$ and $\mathbf{P}_{\mathbf{a},\mathbf{m}}(\mathbf{C}')$, assuming that we have no upper bound, i.e., $\psi \equiv \infty$. We start with the case of fixed end derivatives, i.e., $C' = C_a$ or $C' = C_{ab}$. Using the expression for $v = P_C(\alpha^T M)$ as given in Theorem 4.6, the Peano equations (3.14) for problem $\mathbf{P}_{\mathbf{i},\mathbf{m}}$ become

$$\begin{aligned} F(\alpha) &= \int_a^b M P_{C_{x'_a}}(\alpha^T M)\, dt - Ky - u \\ &= \sum_{l=1}^{L} \int_{a_l}^{b_l} (\alpha^T M + c_l)\, M(t)\, dt \\ &\quad + \sum_{l=0}^{L} \int_{b_l}^{a_{l+1}} \varphi'(t)\, M(t)\, dt - Ky - u = 0. \end{aligned} \tag{5.1}$$

Here $b_0 = t_1 = a_1$ if $t_1 \in E_-$ (i.e. the constraint is inactive at $t = t_1$) and $b_0 = t_1 < a_1$ else. Similarly $a_{L+1} = t_{n+2} = b_L$ if $t_{n+2} \in E_-$ and $a_{L+1} = t_{n+2} > b_L$ else.

For the numerical solution of (5.1) the following result is needed.

LEMMA 5.1. *Let the assumptions of Theorem 4.6 be valid and suppose further that $a_{l+1}(\alpha) > b_l(\alpha)$ for all l. Then $F(\alpha)$ is continuously differentiable and the derivative is given by*

$$F'(\alpha) = T(\alpha) + G(\alpha) + H(\alpha),$$

where

$$t_{ij} = \sum_{l=1}^{L} \int_{a_l}^{b_l} M_i M_j\, dt, \tag{5.2}$$

$$g_{ij} = -\sum_{l=1}^{L'} \frac{1}{I_l} \int_{a_l}^{b_l} M_i\, dt \int_{a_l}^{b_l} M_j\, dt, \tag{5.3}$$

$$h_{ij} = \sum_{l=0}^{L} M_i(a_{l+1})\, \varphi'(a_{l+1}) \frac{\partial a_{l+1}}{\partial \alpha_j} - \sum_{l=0}^{L} M_i(b_l)\, \varphi'(b_l) \frac{\partial b_l}{\partial \alpha_j} \tag{5.4}$$

with $I_l = b_l - a_l$, $L' = L$ if $c_L > 0$, $L' = L - 1$ else.

Proof. We first note, by Theorem 4.6, that the numbers, c_l, a_l, and b_l are determined from the equations

$$\begin{aligned} &f_l = 0, \qquad l = 1, 2, ..., L-1 \\ &f_L \geqslant 0, \end{aligned} \tag{5.5}$$

where

$$f_l = \int_{a_l}^{b_l} (\alpha^{\mathrm{T}} M + c_l)\, dt + \bar{\varphi}(a_l) - \varphi(b_l) \tag{5.6}$$

and

$$\bar{\varphi}(a_l) = \begin{cases} x'_a & \text{if } \ l = 1 \ \text{ and } \ t_1 \in E_-, \\ \varphi(a_l) & \text{else.} \end{cases}$$

Equations (5.5) have unique differentiable solutions $c_l(\alpha)$, $a_l(\alpha)$, and $b_l(\alpha)$. Existence and uniqueness follow from Theorems 2.1 and 4.6 and the differentiability from the assumption $a_{l+1}(\alpha) > b_l(\alpha)$. Differentiating (5.5) with respect to α yields

$$\frac{\partial f_l}{\partial \alpha_j} + \frac{\partial f_l}{\partial c_l} + \frac{\partial f_l}{\partial b_l}\frac{\partial b_l}{\partial \alpha_j} + \frac{\partial f_l}{\partial a_l}\frac{\partial a_l}{\partial a_j} = 0.$$

Combining this equation with (5.6) we can verify (also using that $P_C(\alpha^{\mathrm{T}} M)$ is continuous) that

$$\frac{\partial c_l}{\partial \alpha_j} = -\frac{1}{I_l}\int_{a_l}^{b_l} M_j\, dt \qquad (c_l > 0). \tag{5.7}$$

The lemma follows by differentiating (5.1) and using (5.7). ∎

Newton's method for solving (5.1) is

$$F'(\alpha^k)\, \alpha^{k+1} = F'(\alpha^k)\, \alpha^k - F(\alpha^k). \tag{5.8}$$

We shall derive a more explicit expression and first note, by (5.5) and (5.6), that

$$c_l = \frac{1}{I_l}\left(\varphi(b_l) - \bar{\varphi}(a_l) - \int_{a_l}^{b_l} \alpha^{\mathrm{T}} M\, dt\right). \tag{5.9}$$

Using (5.9) and (5.1)–(5.4) we have

$$\begin{aligned} \int_a^b M P_{C_{x'_a}}(\alpha^{\mathrm{T}} M)\, dt &= T(\alpha)\, \alpha + G(\alpha)\, \alpha \\ &+ \sum_{l=1}^{L} \frac{1}{I_l}(\varphi(b_l) - \bar{\varphi}(a_l)) \int_{a_l}^{b_l} M(t)\, dt + \sum_{l=0}^{L} \int_{b_l}^{a_{l+1}} \varphi' M(t)\, dt. \end{aligned} \tag{5.10}$$

By (5.1)–(5.4), (5.8), and (5.10) we have

LEMMA 5.2. *Consider problem* $\mathbf{P}_{\mathbf{i},\mathbf{m}}(\mathbf{C}')$ *with* $C' = C_a$ *or* $C' = C_{ab}$, $\varphi = \text{constant}$ *and* $\psi \equiv \infty$. *Then Newton's method for solving the Peano equations* (5.1) *for* $\alpha \in \mathbf{R}^{n+1}$ (*or* $\mathbf{R}^{n+2}$) *becomes*

$$(T(\alpha^k) + G(\alpha^k))\,\alpha^{k+1} = Ky + u - \frac{1}{I_1}(\varphi(b_1) - \bar{\varphi}(a_1)) \int_{a_1}^{b_1} M(t)\,dt. \quad (5.11)$$

Remark 5.3. Note that if $L = 1$ and $c_1 = 0$ the G-matrix drops out from (5.11) and we are left with the equations for the unconstrained spline problem.

LEMMA 5.4. *The matrix* $T(\alpha) + G(\alpha)$ *is symmetric and positive semi-definite. If* $|\{t : \sum \beta_i M_i = \text{constant}\}| = 0$ *or* $c_L = 0$ *then* $T(\alpha) + G(\alpha)$ *is positive definite for all* α.

Proof.

$$\sum_{i,j} (t_{ij} + g_{ij})\,\beta_i\beta_j = \sum_{l=1}^{L'} \left[\int_{a_l}^{b_l} \left(\sum \beta_i M_i \right)^2 dt - \frac{1}{I_l} \left(\int_{a_l}^{b_l} \sum \beta_i M_i\,dt \right)^2 \right]$$
$$+ (L - L') \int_{a_L}^{b_L} \left(\sum \beta_i M_i \right)^2 dt \geqslant 0$$

by applying Cauchy–Schwarz inequality to the first sum. Since equality occurs for $\sum \beta_i M_i = \textit{constant}$ the second conclusion follows. Finally, if $c_L = 0$ then $L - L' = 1$. ∎

Concerning Newton's method the following properties are well known.

LEMMA 5.5. *Newton's method converges at a superlinear rate to the solution* α^* *of* $F(\alpha) = 0$ *if*

(i) $F'(\alpha)$ *is continuous in a neighbourhood of the solution.*

(ii) $F'(\alpha^*)$ *is invertible.*

(iii) *The initial value* α^0 *is chosen close enough to* α^*.

Moreover the method converges at a quadratic rate if also

(iv) $F''(\alpha)$ *is bounded in a neighbourhood of* α^*.

COROLLARY 5.6. *Assume that the solution of* (5.1) *fullfils*

(a) $a_{l+1}(\alpha^*) > b_l(\alpha^*) \qquad \forall l$

(b) $\left| \left\{ t : \sum \alpha_j^* M_j = \text{constant} \right\} \right| = 0 \qquad$ *or* $\qquad c_L(\alpha^*) = 0.$

Then if α^0 is chosen close enough to α^*, the iterates $\{\alpha^k\}$ of method (5.11) converge toward α^* at an asymptotic rate which is at least quadratic.

Proof. The assumption (a) implies that $F'(\alpha)$ is continuous in a neighbourhood of α^*. The assumption (b) implies that $F'(\alpha^*)$ is invertible. Finally,

$$F''_{ijk} = \frac{\partial}{\partial \alpha_k}(F'_{ij}) = \frac{\partial}{\partial \alpha_k}(t_{ij}(\alpha) + g_{ij}(\alpha)).$$

It can be verified that this last expression is a bounded function of α in some neighbourhood of α^* (we omit the details). ∎

We now consider the smoothing problem $\mathbf{P}_{\mathbf{a},\mathbf{m}}(\mathbf{C}')$, with $C' = C_a$ or $C' = C_{ab}$. Let

$$F_1(\alpha) = \int_a^b M(t)\, P_C(\alpha^{\mathrm{T}} M)\, dt. \tag{5.12}$$

Then Eqs. (3.16) can be written (also using (3.15))

$$\begin{aligned} F_1(\alpha) + pKQ^{-1}K^{\mathrm{T}}\alpha - pKQ^{-1}A^{\mathrm{T}}\beta &= Ky + u, \\ -pAQ^{-1}K^{\mathrm{T}}\alpha + pAQ^{-1}A^{\mathrm{T}}\beta &= d - Ay. \end{aligned} \tag{5.13}$$

It may be verified easily that Newton's method applied to (5.13) is

$$(G_1^k + G_2)\begin{bmatrix} \alpha^{k+1} \\ \beta^{k+1} \end{bmatrix} = \begin{bmatrix} F_1'(\alpha^k)\,\alpha^k - F_1(\alpha^k) + Ky + u \\ d - Ay \end{bmatrix}, \tag{5.14}$$

where

$$G_1^k = \begin{bmatrix} F_1'(\alpha^k) & 0 \\ 0 & 0 \end{bmatrix}, \qquad G_2 = \begin{bmatrix} \tilde{K} \\ -\tilde{A} \end{bmatrix} [\tilde{K}^{\mathrm{T}}, -\tilde{A}^{\mathrm{T}}] \tag{5.15}$$

and

$$\tilde{K} = \sqrt{p}\, KQ^{-1/2}, \qquad \tilde{A} = \sqrt{p}\, AQ^{-1/2}.$$

Note that G_2 is positive semidefinite. Further we have

LEMMA 5.7. *G_2 is positive definite if and only if*

$$R(\tilde{A}^{\mathrm{T}}) \cap R(\tilde{K}^{\mathrm{T}}) = \varnothing.$$

Remark 5.8. *In the special case that $m = 0$ then, since K has full rank, G_2 is always positive definite.*

COROLLARY 5.9. *Consider problem* $\mathbf{P}_{\mathbf{a},\mathbf{m}}(\mathbf{C})$ *with* $C' = C_a$ *or* $C' = C_{ab}$, $\varphi = \text{constant}$ *and* $\psi \equiv \infty$. *Also assume that the condition* $Az = d$ *is not present. Then Newton's method for solving the Peano equations* (5.13) *for* $\alpha \in \mathbf{R}^{n+1}$ (*or* $\mathbf{R}^{n+2}$) *becomes*

$$\begin{aligned}(T(\alpha^k) + G(\alpha^k) + pKQ^{-1}K^{\mathrm{T}})\,\alpha^{k+1}& \\ = Ky + u - \frac{1}{I_1}(\varphi(b_1) - \bar{\varphi}(a_1)) \int_{a_1}^{b_1} M(t)\,dt.& \qquad (5.16)\end{aligned}$$

COROLLARY 5.10. *Assume that the solution of* (5.13) *fulfills*

$$a_{l+1}(\alpha^*) > b_l(\alpha^*), \qquad \forall l.$$

Then if α^0 *is chosen close enough to* α^*, *the iterates* $\{\alpha^k\}$ *of method* (5.16) *converge toward* α^* *at an asymptotic rate which is at least quadratic.*

We now study briefly the case with free end derivatives.

LEMMA 5.11. *Consider problem* $\mathbf{P}_{\mathbf{i},\mathbf{m}}(\mathbf{C}')$ *with* $C' = W^2(a, b)$, $\psi \equiv \infty$, *and* $\varphi = \text{constant}$. *Then Newton's method for solving the Peano equations* (3.20) *for* $\alpha \in \mathbf{R}^{n+1}$ *and* $x'_a \in \mathbf{R}$ *becomes*

$$\begin{bmatrix} T(\alpha^k) + G(\alpha^k) & W \\ W^{\mathrm{T}} & -1/I_1 \end{bmatrix} \begin{bmatrix} \alpha^{k+1} \\ x_a'^{k+1} \end{bmatrix} = \begin{bmatrix} Ky - (1/I_1)\,\varphi(b_1) \int_{a_1}^{b_1} M\,dt \\ -c_1^k - (1/I_1)\,x_a'^k - (1/I_1) \int_{a_1}^{b_1} \alpha^{k^{\mathrm{T}}} M\,dt \end{bmatrix},$$

assuming $t_1 \in E_-$ (*i.e.*, $x'_a > \varphi(a)$). *Here* $W = -u_0 - (1/I_1) \int_{a_1}^{b_1} M\,dt$.

Proof. Differentiate (3.20), using (5.10), with respect to α (use Lemma 5.1) and x'_a. Use that (in (3.20)) $f(t_1) = \alpha_0 M_0(t_1) + c_1$ and obtain $\partial c_1/\partial\alpha$ from (5.7), $\partial c_1/\partial x'_a$ from (5.9). Putting the derived results into the Newton equations for (3.20) gives the above iteration. ∎

Remark 5.12. The Jacobian matrix J in the above iteration is no longer positive definite ($J_{n+2,n+2} = -1/I_1 < 0$). However, in our computer experiments we still obtain good convergence properties (e.g., quadratic convergence).

We leave it to the interested reader to write down the corresponding Newton iteration for problem $\mathbf{P}_{\mathbf{a},\mathbf{m}}(\mathbf{C}')$, $C' = W^2(a, b)$.

6. NUMERICAL RESULTS

We first give a brief description of the computer implementation of the Newton schemes. At each iteration step k, the projection $P_{C_{x'_a}}(\alpha^{k^{\mathrm{T}}} M)$ is computed (by the algorithm in Section 4), producing the numbers $\{a_l^k, b_l^k, c_l^k\}$. Then the matrices T and G are formed. The integrals occurring in T and G are evaluated exactly using Simpson's rule. T is a symmetric, tridiagonal matrix. The matrix G is also symmetric but has a more complex structure. Note that there are at most two terms in the sum defining g_{ij}, (5.3), because $\text{supp}(M_i) = [t_i, t_{i+2}]$ and there are at most two new knots in any interval $[t_j, t_{j+1}]$. The matrix G therefore has a block structure (the numbers of blocks is equal to L). For an illustration, see Figure 2b. We solve the linear system in Newton's method by Gaussian elimination. Note that pivoting is not needed for the case with given end derivatives. Once the Newton iteration has converged the second derivative, $x''(t)$, is recovered (using (iii), $u = \alpha^{\mathrm{T}} M$, and (iv) in Theorem 4.6, with $\varphi' = 0$, in our case) and stored as a piecewise linear continuous function.

We now discuss two ways of obtaining $x(t)$ from $x''(t)$. In method 1, at all knots $\bar{t}_j$, which coincide with with an original t_j-knot, interpolation is done using y_j (or z_j in the case of smoothing). At other knots continuity of x and x' provides the necessary equations. This procedure is described in detail in [1].

In method 2 the given (or computed) value of x'_a is used. Simply integrate the first segment of $x''(t)$ from $t = t_1$ and use y_1 (or z_1) and x'_a as initial values. Then proceed sequentially over all segments.

The two integration methods distribute possible errors in the coefficients α_k quite differently. By construction, method 2 will produce a solution $x(t)$ belonging to $C^2(a, b)$. However, $x(t)$ will, in case of errors in α_k, not satisfy the interpolation conditions exactly. On the other hand, method 1, by construction, always interpolates correctly at $\{\bar{t}_j\}$. However, if the Peano equations are only approximately satisfied, $x'(t)$ will fail to be continuous at $\{\bar{t}_j\}$.

The choice of p and Q should be dictated by the noise component in the data vector y. One possibility is to use cross-validation for estimating p and Q [29]. We have adopted this technique in another context (a nonlinear programming problem) [10]. It is quite obvious that the same approach could be used here. We will however not pursue this in the present paper. Instead we have taken

$$q_{ii} = 1/h^3, \qquad q_{ij} = 0, \qquad i \neq j, \qquad h = \max_i |t_{i+1} - t_i|,$$

using a dimension argument. The value of p was varied in the tests.

We conclude this section by presenting the results from a few numerical tests. These were all run in double precision (with a Fortran compiler) on a SUN workstation. As error measure in the Newton iteration we used

$$\text{err} = \max_j \frac{|\alpha_j^{k+1} - \alpha_j^k|}{|\alpha_j^k| + 10^{-10}}.$$

In the figures we have listed the number of iterations needed for err $< 10^{-10}$. In several cases, due to the quadratic convergence, err $\sim 10^{-15}$ As start value we picked an α^0 such that $P_C(\alpha^{0^T}M) = \alpha^{0^T}M$; i.e., the next iterate α^1 is associated with the unconstrained spline ($\alpha^0 = (1, 1, .., 1)^T$ was used throughout).

We present tests for either a given value of $x'(a)$ ($x'(a)$ was approximated by $(y_2 - y_1)/(t_2 - t_1)$), Figs. 4, 4, 6; or free end derivatives, Fig. 5. Figure 3 contains plots of monotone reconstructions of the RPN-14 data of [13] for $p = 0$ ($p = 0$ corresponds to interpolation; cf. (5.11) and (5.16)) and $p = 1$ (smoothing). Only the reconstruction up to $t = 11$ is shown. From then on the two curves are almost identical and constant (for $p = 0$ in the interval [11.99, 15.9], $|x''(t)|$ is less than 10^{-4}). For $p = 0$ the two first active intervals are picked up in the early iterations whereas the last one occurs for the first time in the seventh iteration. The quadratic convergence starts at iteration 11 (there err ~ 0.1).

The next data set is a slight modification of the previous one. Now $x(12) = 0.975$, $x(15) = 0.965$, $x(20) = 0.990$, and all other values are identical to the RPN-14 data. The modification means that the dataset no longer corresponds to sampling a monotone function (and hence interpolation using $\varphi = 0$ is no longer possible). In Figure 4 the reconstruction using $\varphi = 0$ and $p = 0.01$ is shown. The reconstruction using the additional constraint $\sum z_i = constant$ was also computed (using (5.14)). However, in this case the effect is simply adding a constant to the reconstruction obtained

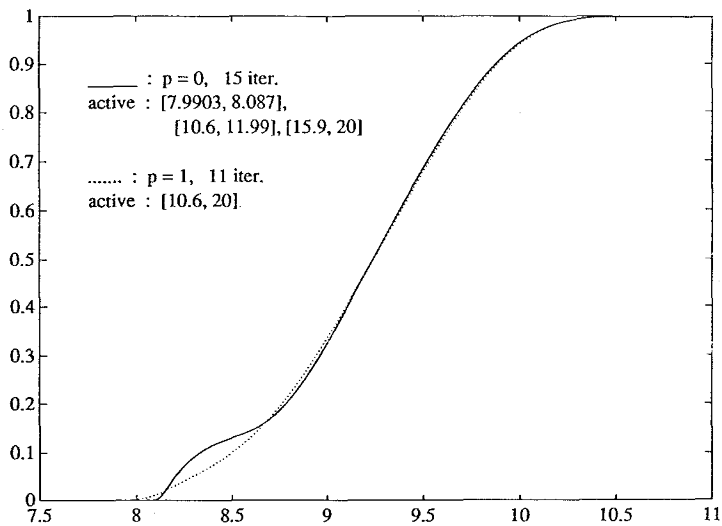

FIG. 3. RPN-data, $x'(t) \geqslant 0$, $x'(a) = 2.76\text{E-}4$.

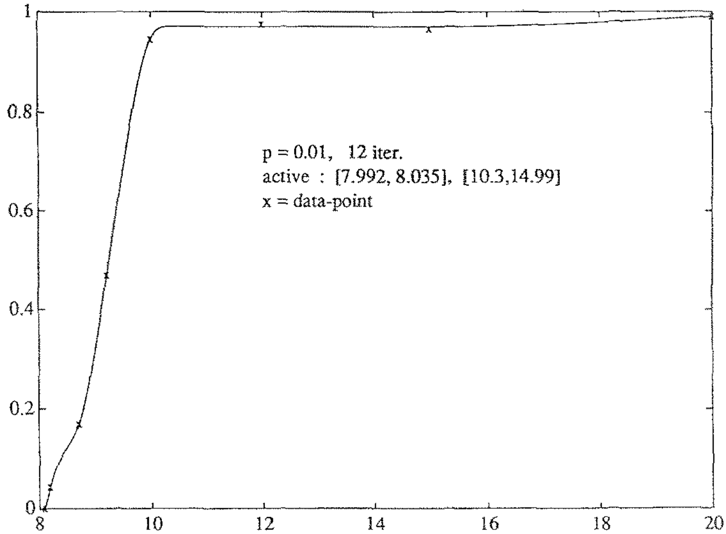

FIG. 4. Modified RPN-data, $x'(t) \geqslant 0$, $x'(a) = 2.76\text{E-}4$.

without the additional constraint. The reason is that $KQ^{-1}A^{T} = 0$ for $A = (1, 1, ..., 1)$ since Q here is a multiple of the identity matrix. Hence the computed x'' is the same for the two reconstructions (cf. (5.13)).

In Fig. 5 we consider Example 1 in [5]. Here x'_a is considered a free variable and the algorithm in Lemma 5.11 is used. A similar run with the

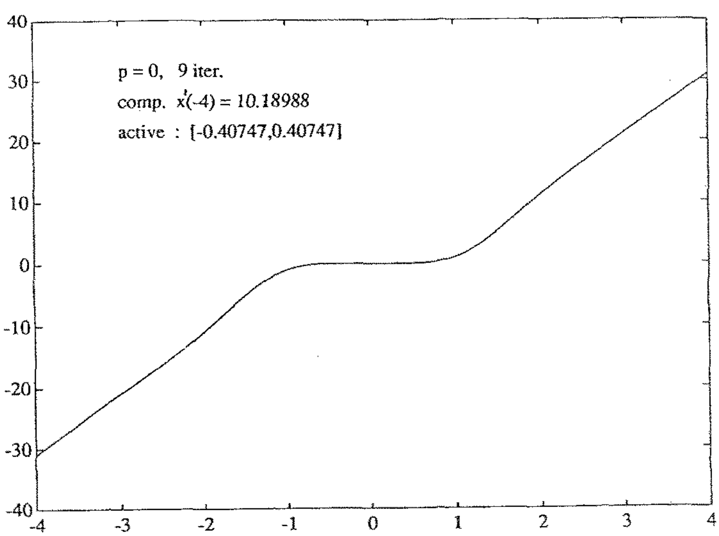

FIG. 5. DR1-data, free end derivatives, $x'(t) \geqslant 0$.

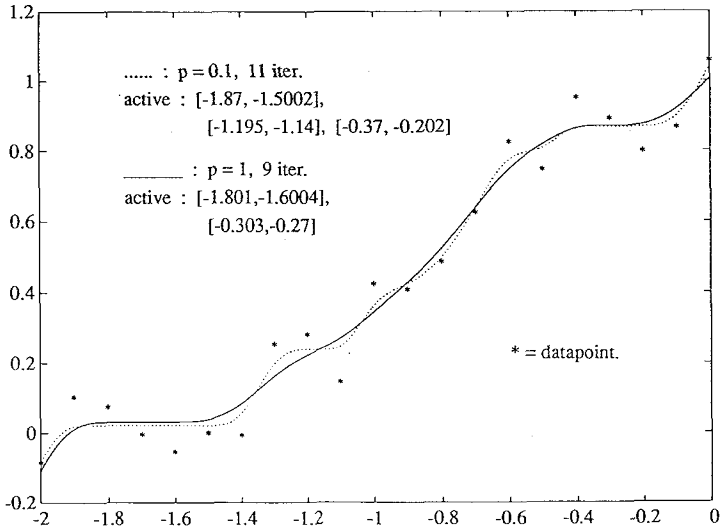

FIG. 6. S-curve with noise, $x'(t) \geqslant 0$, $x'(a) = 1.88$.

RPN-data reveals that $x'(a) = \varphi(a) = 0$ is the value corresponding to natural boundary conditions (cf. Theorem 3.9).

Finally, we have corrupted the function $\exp(-x^2)$(an "S-curve") with additive noise. Figure 6 shows reconstructions for two values of the smoothing parameter p.

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