Best near-interpolation by curves: optimality conditions

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Abstract

A parametric curve $f \in L_2^{(m)}([0\,.\,.1] \longrightarrow \mathbb{R}^d)$ is a near-interpolant to prescribed data points $z_{ij} \in \mathbb{R}^d$ at data sites t_i, $0{=}t_1{\le}t_2{\le}\cdots{\le}t_n{=}1$, and within tolerances $0 < \varepsilon_{ij} \le \infty$, if $|f^{(j-1)}(t_i) - z_{ij}| \le \varepsilon_{ij}$ for $i{=}1{:}n$ and $j{=}1{:}m$. In this paper, optimality conditions are derived for those near-interpolants that minimize $\int_0^1 |f^{(m)}|^2$. We consider both fixed and free data sites, with the possibility of repetitions. For fixed data sites the problem is convex, and we obtain a full characterization for the minimizers (i.e., a necessary and sufficient optimality condition); for free data sites the problem is non-convex, and we obtain a first-order necessary condition. These conditions are applied to the computation of best near-interpolants in [K99c].

1. Introduction

The goal in the variational problem of "best near-interpolation" is to obtain the "smoothest" possible parametric curves that meet prescribed data to within local bounds on the error from interpolation. Near-interpolation is particularly beneficial when there is noise or randomness in the data, situations that often cause problems in curve fits. Moreover, there is a natural mechanism in near-interpolation (via active and inactive constraints) for selecting an optimal sequence of data sites that is often smaller than the given sequence of data points. This is beneficial since the minimizers are polynomial splines and a reduction in the number of data sites means a reduction in the number of polynomial pieces. Since we are considering curves here, the data sites are the parameter locations at which the curves meet the data and may vary from curve to curve. Hence, to include all parametrizations, the data sites are allowed to vary in the most general case.

The setup is as follows. We say that a **curve** $f : [0\,.\,.1] \longrightarrow \mathbb{R}^d$ in some normed linear space X is a **near-interpolant** to prescribed **data** $z \in Z$ within **tolerances** ε and with respect to a **data map** $\Lambda_t : X \longrightarrow Z$ if $\Lambda_t f \in B_\varepsilon^-(z)$ for a particular neighborhood $B_\varepsilon^-(z)$ of z. Here, $X := L_2^{(m)}([0\,.\,.1] \longrightarrow \mathbb{R}^d)$ is the Sobolev space of vector-valued functions (curves) f such that $f^{(m)}$ is in the Lebesgue space $Y := L_2([0\,.\,.1] \longrightarrow \mathbb{R}^d)$, $m \ge 1$. In particular, the curves in X have $m{-}1$ continuous derivatives. The data map

$$\Lambda_t : X \longrightarrow Z := (\mathbb{R}^{m \times n})^d : f \longmapsto (\lambda_{ij} f := f^{(j-1)}(t_i) : i{=}1{:}n,\ j{=}1{:}m) \tag{1.1}$$

is then continuous on X for any sequence of **data sites**

$$t \in \Delta_n^- := \{t \in \mathbb{R}^n : 0{=}t_1{\le}t_2{\le}\cdots{\le}t_n{=}1\},$$

and is moreover *onto* when the data sites are strictly increasing, i.e., when

$$t \in \Delta_n := \{t \in \mathbb{R}^n : 0{=}t_1{<}t_2{<}\cdots{<}t_n{=}1\}.$$

For prescribed sequences of data $z = (z_{ij})$ and tolerances $\varepsilon = (\varepsilon_{ij})$ with $0 < \varepsilon_{ij} \leq \infty$, let

$$B_\varepsilon^-(z) := \underset{ij}{\times} B_{\varepsilon_{ij}}^-(z_{ij}),$$

with $B_{\varepsilon_{ij}}^-(z_{ij})$ the closed Euclidean ball of radius ε_{ij} in $\mathbb{R}^d$. Hence, $\Lambda_t f \in B_\varepsilon^-(z)$ when $|\lambda_{ij} f - z_{ij}| \leq \varepsilon_{ij}$ for all i and j. This generalizes interpolation where $\Lambda_t f = z$. In particular, $\lambda_{ij} f \approx z_{ij}$ when ε_{ij} is small – hence the term "near-interpolant". Note that the monotonicity of the data sites forces the curves to meet the data points z_{ij} in the order in which they appear in the sequence z.

For a given functional $J : X \longrightarrow \mathbb{R}$, we say that f is a **best near-interpolant** for fixed data sites t if it solves the minimization problem

$$(A) \qquad \underset{f \in X}{\text{minimize}} \ \{J(f) : \Lambda_t f \in B_\varepsilon^-(z)\},$$

and for free data sites if (f, t) solves

$$(B) \qquad \underset{f \in X,\ t \in \Delta_n^-}{\text{minimize}} \ \{J(f) : \Lambda_t f \in B_\varepsilon^-(z)\}.$$

Here, J is the standard quadratic functional

$$J : X \longrightarrow \mathbb{R} : f \longmapsto \int_0^1 |f^{(m)}(s)|^2 \, \mathrm{d}s,$$

a semi-norm on X.

In this paper, optimality conditions are derived for the solutions to (A) and (B). For (A), the data sites are fixed. As a consequence, the problem is convex, and we obtain full characterizations (i.e., necessary and sufficient optimality conditions) for the solutions. We first derive an abstract characterization by the method of Lagrange, stated in Theorem 4.2, and second, with the solutions known to be polynomial spline curves, we give a finite-dimensional characterization that is useful for computation, stated in Theorem 5.8. The connection between these characterizations is made by a result stated in Lemma 5.3, part (ii). We also state conditions for the existence and uniqueness of solutions to problem (A).

With the data sites free to vary, problem (B) is not convex, and we obtain a first-order necessary optimality condition for the (local) solutions. As in problem (A), the solutions to (B) are spline curves. Hence, to obtain a necessary condition, the minimization in problem (B) is restricted to a certain subset of splines in X that is parametrized by the coefficients and breakpoints (i.e., data sites) of the spline curves. The parametrization is defined with respect to the spline basis dual to Λ_t, for each t, which is particularly convenient since the constraints in (B) become independent of the data sites. Hence, in this parametrization, J can be varied "freely" with respect to the data sites without affecting the feasibility of the curves. The results of this variation are stated in Lemma 7.3 and Proposition 7.5, and the necessary condition is stated in Theorem 7.9. As with the optimality conditions derived for problem (A), the necessary condition for the solutions to (B) apply in the case of repeated data sites, i.e., when $t_i = t_{i+1}$ for some i. The existence of solutions to problem (B) is investigated in [K99b].

For the case that $d = 1$, problem (A) is similar to the problem

$$(1.2) \qquad \underset{f \in X}{\text{minimize}} \ \{J(f) : a_{ij} \leq \lambda_{ij} f \leq b_{ij}\}$$

of "best interpolation with inequality constraints", as studied, for example, in [A67], [L69], [MS69], [CP78] and [AE95], in more or less generality. As a consequence, the characterization obtained here is similar to that in these papers, with, in particular, the extension to curves here. The connection between problems (1.2) and (A) is discussed further in [K99d].

Problem (B) is similar to the problem of "best interpolation by curves", to which (B) reduces when $\varepsilon_{ij} = 0$. This was studied in [To82], [M84], [SeSi86], [RaSe88] and [Se97] for data maps of the form $f \longmapsto f(t_i)$ (i.e., $\varepsilon_{ij} = \infty$ for $j > 1$ in the setup here), in which case the minimizers are "natural spline curves" in C^m. In particular, for $m = 2$, a necessary optimality condition is derived in [To82] (as described in detail in [To98]) based on the calculus of variations. Since their curves are C^2 and their interpolation conditions are of the form $f \longmapsto f(t_i)$, those results do not directly apply here. Hence, the variational method used here is different. For the problem of interpolation, existence and uniqueness are verified when $m = 2$ and $d = 1$ in [M84], existence is verified for $m \geq 1$ and $d \geq 1$ in [SeSi86], and uniqueness is investigated in [Se97] in the case that $m = 2$ and $d \geq 1$. The existence results in [SeSi86] are extended to the problem of near-interpolation in [K99b].

2. Additional notation

The following notation will be used in the remainder of this paper. Let D be the derivative operator for functions in X. Then D^m is m-fold differentiation, and in particular $D^m f = f^{(m)}$ and $D^m X = Y$. The kernel of D^m, denoted $\ker D^m$, is the linear space of those functions in X whose restriction to $[0..1]$ is a polynomial (curve) of **order** m, i.e., of degree $< m$.

Let

$$\langle f, g \rangle_X := \underbrace{\sum_{j=1}^{m} f^{(j-1)}(0) \cdot g^{(j-1)}(0)}_{\langle f, g \rangle_{\ker D^m}} \; + \; \underbrace{\int_0^1 f^{(m)}(s) \cdot g^{(m)}(s) \, \mathrm{d}s}_{\langle f^{(m)}, g^{(m)} \rangle_Y}$$

be inner products on X, $\ker D^m$ and Y, respectively, with $u \cdot v$ denoting the standard dot product on $\mathbb{R}^d$. Norms are defined in the usual way:

$$\|f\| := \langle f, f \rangle^{1/2}.$$

With this, X becomes a complete inner product space (i.e., a Hilbert space). Note in particular that

$$J(f) \;=\; \|f^{(m)}\|_Y^2,$$

which is the square of a seminorm on X. On Z we have the inner product

$$\langle \alpha, \beta \rangle_Z := \sum_{i=1}^{n} \sum_{j=1}^{m} \alpha_{ij} \cdot \beta_{ij}.$$

The optimality conditions derived in this paper depend on certain sequences of "weights" $w = (w_{ij})$ (i.e., "Lagrange multipliers") with $w_{ij} \in \mathbb{R}$ for each i and j. These act on sequences $\alpha = (\alpha_{ij})$ in Z by

$$w\,\alpha := (w_{ij}\alpha_{ij} : i{=}1{:}n,\; j{=}1{:}m)$$

with $\alpha_{ij} \in \mathbb{R}^d$ for each i and j, and hence on the maps Λ_t by

$$w\,\Lambda_t : X \longrightarrow Z : f \longmapsto w\,(\Lambda_t f).$$

The solutions to (A) and (B) are in the linear space

$$\$_{2m,t} := \$_{2m,t}([0\,..1] \longrightarrow \mathbb{R}^d) \tag{2.1}$$

of piecewise polynomial *curves* on $[0\,..1]$, into $\mathbb{R}^d$, of order $2m$, and with $m-1$ continuous derivatives at the "breakpoints" t_i in t. On $\$_{2m,t}$, let

$$\begin{aligned}
&f(t_i^+) := \lim_{t\downarrow t_i} f(t), \qquad f(t_i^-) := \lim_{t\uparrow t_i} f(t),\\
&\lambda_{ij}^{\pm} : f \longmapsto f^{(j-1)}(t_i^{\pm}),\\
&\mathrm{jmp}_{t_i} : f \longmapsto f(t_i^+) - f(t_i^-),\\
&\Psi_t : f \longmapsto ((-1)^{m+j-1}\mathrm{jmp}_{t_i} f^{(2m-j)} : i{=}1{:}n,\ j{=}1{:}m).
\end{aligned} \tag{2.2}$$

To accommodate the "jump maps" at $t_1 = 0$ and $t_n = 1$, we specify that $f^{(j-1)}(0^-){:=}0{=:}f^{(j-1)}(1^+)$.

The optimality conditions in Theorem 4.2 are stated in terms of the adjoint operators $\lambda_{ij}^* : \mathbb{R}^d \longrightarrow X$, $\Lambda_t^* : Z \longrightarrow X$ and $D^{m*} : Y \longrightarrow X$, with $X = X^*$ and $Z = Z^*$ under the usual isometric isomorphisms. In particular, λ_{ij}^* is associated with the representer of λ_{ij}, and

$$\Lambda_t^* : \alpha \longmapsto \sum_{ij} \lambda_{ij}^* \alpha_{ij}.$$

It is convenient for deriving the optimality conditions to write the constraints in (A) and (B) in terms of inequalities. For this, let

$$\Gamma_t : X \longrightarrow \mathbb{R}^{m\times n} : f \longmapsto (\Gamma_{ij}(f) : i{=}1{:}n,\ j{=}1{:}m)$$

with

$$\Gamma_{ij} : X \longrightarrow \mathbb{R} : f \longmapsto |\lambda_{ij} f - z_{ij}|^2,$$

and let $\varepsilon^2 := (\varepsilon_{ij}^2 : i{=}1{:}n,\ j{=}1{:}m)$. Then, problems (A) and (B) can be restated as

$$\operatorname*{minimize}_{f\in X}\ \{J(f) : \Gamma_t(f) \le \varepsilon^2\} \tag{2.3}$$

for fixed $t \in \Delta_n^-$, and

$$\operatorname*{minimize}_{f\in X,\ t\in\Delta_n^-}\ \{J(f) : \Gamma_t(f) \le \varepsilon^2\}, \tag{2.4}$$

respectively.

3. Existence of the solutions to problem (A)

Theorem 3.1. *Assume that $\Lambda_t^{-1}B_\varepsilon^-(z) \neq \emptyset$. Then, solutions to (A) exist, and all solutions are mapped by D^m to the same function.*

Proof: Since $\Lambda_t^{-1}B_\varepsilon^-(z)$ is not empty, its image $D^m(\Lambda_t^{-1}B_\varepsilon^-(z))$ is not empty. Moreover, $\Lambda_t^{-1}B_\varepsilon^-(z)$, as the inverse image of a convex set under a linear map, is convex, hence so is its linear image $D^m(\Lambda_t^{-1}B_\varepsilon^-(z))$. Further, as the inverse image of a closed set under a bounded linear map, $\Lambda_t^{-1}B_\varepsilon^-(z)$ is closed, hence so is its image $D^m(\Lambda_t^{-1}B_\varepsilon^-(z))$ since D^m is a bounded linear map (since $\|D^m f\|_Y \leq \|f\|_X$) from a Banach space *onto* a Banach space, hence an open map (by the Open Mapping Theorem).

By a standard theorem on projections in Hilbert spaces, the nonempty, closed and convex set $D^m(\Lambda_t^{-1}B_\varepsilon^-(z))$ contains a *unique* element h of minimal norm. Since $J = \|D^m(\cdot)\|_Y^2$, then η solves (A) iff $\eta \in \Lambda_t^{-1}B_\varepsilon^-(z)$ and $D^m\eta = h$. □

Proposition 3.2. *Let $t \in \Delta_n$. Then $\Lambda_t : X \longrightarrow Z$ is onto and $\Lambda_t^* : Z \longrightarrow X$ is 1-1.*

Proof: When $t \in \Delta_n$, it is easy to find $f \in X$ such that $\Lambda_t f = \alpha$ for any $\alpha \in Z$. Indeed, there is a unique piecewise polynomial (curve) of order $2m$ that satisfies this condition. Hence, Λ_t maps X onto Z. Since the dimension of Z is finite, it follows that $\Lambda_t^* : Z \longrightarrow X$ is 1-1. □

Corollary 3.3. *Solutions to (A) exist when $t \in \Delta_n$, or when $t \in \Delta_n^-$ and $B_{\varepsilon_{ij}}^-(z_{ij}) \cap B_{\varepsilon_{i+1,j}}^-(z_{i+1,j}) \neq \emptyset$ for j=1:m when $t_i = t_{i+1}$.*

Proof: By Proposition 3.2, $\Lambda_t f = z$ for some $f \in X$ when $t \in \Delta_n$, implying, in particular, that $\Lambda_t^{-1}B_\varepsilon^-(z)$ is not empty. On the other hand, when $t \in \Delta_n^-$ and there are repeated data sites, then, with $t' := (t_i : t_i \neq t_{i-1})$ the maximal strictly increasing subsequence of t, $\Lambda_{t'}$ maps X 1-1 and onto *its* range. Then $\Lambda_{t'} f = \hat{z}$ for some $f \in X$, with $\hat{z} \in B_\varepsilon^-(z)$ defined such that $\hat{z}_{ij} = \hat{z}_{i+1,j}$ when $t_i = t_{i+1}$, which necessarily exists by the assumption that $B_{\varepsilon_{ij}}^-(z_{ij}) \cap B_{\varepsilon_{i+1,j}} \neq \emptyset$. Hence, again, $\Lambda_t^{-1}B_\varepsilon^-(z)$ is not empty, and by Theorem 3.1, minimizers exist. □

4. An abstract characterization of the solutions to (A)

The functional J and the feasible set $\Lambda_t^{-1}B_\varepsilon^-(z)$ for Problem (A) are convex. Hence, the optimality conditions derived here are an infinite-dimensional extension of the so-called Kuhn-Tucker conditions. These are particularly easy to derive when problem (A) is written as in (2.3) since J and Γ_{ij} are Frechét differentiable functions. Indeed, the derivatives of J and Γ_{ij} at $\eta \in X$ are given by the maps

$$DJ(\eta) : f \longmapsto 2\langle D^m\eta, D^m f\rangle_Y = \langle \nabla J(\eta), f\rangle_X$$

and

$$D\Gamma_{ij}(\eta) : f \longmapsto 2\langle \lambda_{ij}\eta - z_{ij}, \lambda_{ij} f\rangle_Z = \langle \nabla\Gamma_{ij}(\eta), f\rangle_X,$$

respectively, with the "gradient" of J at η given by

$$\nabla J(\eta) := 2\, D^{m*} D^m \eta$$

and the gradient of Γ_{ij} at η given by

$$\nabla \Gamma_{ij}(\eta) := 2\, \lambda_{ij}^{*}(\lambda_{ij}\eta - z_{ij}),$$

which are the representers for $DJ(\eta)$ and $D\Gamma_{ij}(\eta)$, respectively (see [BP78: page 93]). (Note that the usage of D in DJ and $D\Gamma_{ij}$ is different than in the maps D and D^m used throughout this thesis.)

For necessity in the characterization of the solutions to (A), we assume the following constraint qualification:

Condition 4.1 (Slater's condition, [BP78: page 157]). *$\Gamma_t(f) < \varepsilon^2$ for some $f \in X$ (equivalently, the interior of $\Lambda_t^{-1} B_\varepsilon^-(z)$ is not empty).*

Condition 4.1 holds in problem (A) when $t \in \Delta_n$, or when $t_i = t_{i+1}$ for some i and the interior of $B_{\varepsilon_{ij}}^-(z_{ij}) \cap B_{\varepsilon_{i+1,j}}^-(z_{i+1,j})$ is not empty for j=1:m (under the standing assumption that $\varepsilon_{ij} > 0$). This is not the case when $B_{\varepsilon_{ij}}^-(z_{ij}) \cap B_{\varepsilon_{i+1,j}}^-(z_{i+1,j})$ consists of a single point in $\mathbb{R}^d$, i.e., when the constraints force "interpolation" at a point. Since the constraint qualification in Condition 4.1 applies only to inequality constraints, the solution in this case is to replace the inequality constraints leading to interpolation by certain equality constraints. This was discussed in [K99a], but is excluded here for simplicity of the exposition.

The characterization stated next is a "Lagrange-type" result. Basically, under the constraint qualification in Condition 4.1, η minimizes (A) iff $\nabla J(\eta)$ is in the span of those $\nabla \Gamma_{ij}(\eta)$ for which $\Gamma_{ij}(\eta) = \varepsilon_{ij}^2$ (i.e, those constraints that are "active").

Theorem 4.2. *Let $t \in \Delta_n^-$, $z \in Z$ and $\varepsilon \in \mathbb{R}_+^{m\times n}$. Assume that Condition 4.1 holds. Let $\eta \in \Lambda_t^{-1} B_\varepsilon^-(z)$.*

(i) If $\ker D^m \cap \Lambda_t^{-1} B_\varepsilon^-(z) = \emptyset$, then η solves (A) iff for some $w \in \mathbb{R}^{m\times n}$

$$\begin{aligned} &D^{m*} D^m \eta + \Lambda_t^* \, w(\Lambda_t \eta - z) = 0, \\ &w \geq 0, \quad w\,(\Gamma_t(f) - \varepsilon^2) = 0. \end{aligned} \tag{4.3}$$

(ii) If $\ker D^m \cap \Lambda_t^{-1} B_\varepsilon^-(z) \neq \emptyset$, then η solves (A) iff $\eta \in \ker D^m$.

Proof: Part (ii) is trivial since $J(\eta) = \|D^m \eta\|_Y^2 = 0$ iff $\eta \in \ker D^m$. Hence, it remains to verify part (i). For this, recall that the functionals J and Γ_{ij} are convex and differentiable on X, with gradients $\nabla J(\eta)$ and $\nabla \Gamma_{ij}(\eta)$ as defined above. It follows by a direct application of [BP78: page 159, Corollary 1.2] that η solves (A) iff

$$\nabla J(\eta) + \sum_{i=1}^{n} \sum_{j=1}^{m} w_{ij}\, \nabla \Gamma_{ij}(\eta) = 0$$

for some $w = (w_{ij})$ in $\mathbb{R}^{m\times n}$ such that $w_{ij} \geq 0$ and $w_{ij}\Gamma_{ij}(f) = 0$ for all i and j. Then, (4.3) follows on setting $\nabla J(\eta) = 2\, D^{m*}D^m\eta$ and

$$\begin{aligned}\sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij}\,\nabla\Gamma_{ij}(\eta) &= \sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij}\,2\,\lambda_{ij}^*(\lambda_{ij}\eta - z_{ij})\\ &= 2\sum_{i=1}^{n}\sum_{j=1}^{m}\lambda_{ij}^*\,w_{ij}\,(\lambda_{ij}\eta - z_{ij})\\ &= 2\,\Lambda_t^*\,w(\Lambda_t\eta - z).\end{aligned}$$

□

5. A finite-dimensional characterization of the solutions to (A)

Theorem 4.2 characterizes the solutions to (A) as solutions to a linear equation in the infinite-dimensional space X. In this section, we first verify by standard means that the solutions are spline curves, and then we derive a finite-dimensional characterization that is useful for computation. The case of repeated data sites (when $t_i = t_{i+1}$ for some i) will require special attention here. For the first few results, we will assume that there are no such repetitions, i.e, that $t \in \Delta_n$.

Proposition 5.1. *Assume that $t \in \Delta_n$. Then,* $\operatorname{ran}(\Lambda_t^*) = \$_{2m,t}$.

Proof: Assume first that $d = 1$. In this case, it is well-known that the "representers" λ_{ij}^* of the functionals λ_{ij} are in $\$_{2m,t}$. Indeed, these representers can be calculated from the "reproducing kernel function" on X (see [W90: p. 8] and [dBL66]). Therefore, $\operatorname{ran}(\Lambda_t^*) = \operatorname{span}(\lambda_{ij}^*) \subset \$_{2m,t}$ in this case. Moreover, it is well-known that the dimension of $\$_{2m,t}$ is $m\,n$. Indeed, each $f \in \$_{2m,t}$ can be uniquely represented by $n-1$ polynomials p_i of order $2m$ (degree $2m-1$) such that $p_i^{(j-1)}(t_i) = f^{(j-1)}(t_i)$ and $p_i^{(j-1)}(t_{i+1}) = f^{(j-1)}(t_{i+1})$ for i=1:n and j=1:m (the so-called two-point Hermite interpolants). Therefore, $\#\lambda_{ij}^* = m\,n = \dim \$_{2m,t}$, and since Λ_t^* is 1-1 (by Proposition 3.2), it follows that $\operatorname{ran}(\Lambda_t^*) = \$_{2m,t}$.

When $d > 1$, the same arguments apply to each component of the vector maps λ_{ij}^*. In this case, $\dim \$_{2m,t} = d\,m\,n$. □

Corollary 5.2. *Assume that $t \in \Delta_n$ and that η solves (A). Then $\eta \in \$_{2m,t}$.*

Proof: If $\ker D^m \cap \Lambda_t^{-1}B_\varepsilon^-(z) {\neq} \emptyset$, then $\eta \in \ker J = \ker D^m \subset \$_{2m,t}$. Hence, assume that $\ker D^m \cap \Lambda_t^{-1}B_\varepsilon^-(z){=}\emptyset$ from here on. Let $\eta =: p + h$ in $\ker D^m \oplus (\ker D^m)^\perp$, an orthogonal sum decomposition of X. Since $h \in (\ker D^m)^\perp$, it follows that

$$\langle D^{m*}D^m h, \cdot\rangle_X = \langle D^m h, D^m\cdot\rangle_Y = \langle h,\cdot\rangle_{\ker D^m} + \langle D^m h, D^m\cdot\rangle_Y = \langle h,\cdot\rangle_X,$$

and so $D^{m*}D^m h = h$. That is, $D^{m*}D^m$ is the identity map on $(\ker D^m)^\perp$. By (4.3)

$$h = D^{m*}D^m\eta = -\Lambda_t^*\,w(\Lambda_t\eta - z).$$

Therefore, $h \in \operatorname{ran}(\Lambda_t^*) = \$_{2m,t}$ (by Proposition 5.1), ans so $\eta = p + h \in \ker D^m + \$_{2m,t} = \$_{2m,t}$. □

In (5.4) of the next result, the value of the J on $\$_{2m,t}$ is stated in terms of the "jump-map" $\Psi_t : X \longrightarrow Z$ defined in (2.2); a standard application of integration by parts. In (5.5), these jump-maps are shown to have a particular abstract representation that provides a useful means to pass from the abstract infinite dimensional problem on X to the finite-dimensional problem on $\$_{2m,t}$, and that is used to derive the characterization stated in Theorem 5.8.

Lemma 5.3. *Let $t \in \Delta_n$ and $f \in \$_{2m,t}$, and let Ψ_t be the "jump-map" from (2.2). Then,*

$$J(f) = \langle \Psi_t f, \Lambda_t f \rangle_Z \tag{5.4}$$

$$\Psi_t f = (\Lambda_t^*)^{-1} D^{m*} D^m f. \tag{5.5}$$

Proof: Since $f \in \$_{2m,t}$, the one-sided derivatives $f^{(j-1)}(t_i^{\pm})$ are defined for all i and j. Let $g \in X$. By integration by parts,

$$\begin{aligned}
\langle D^m f, D^m g \rangle_Y &= \int_0^1 f^{(m)} \cdot g^{(m)} = \sum_{i=1}^{n-1} \int_{t_i}^{t_{i+1}} f^{(m)} \cdot g^{(m)} \\
&= \sum_{i=1}^{n-1} \sum_{j=1}^{m} (-1)^{j-1} f^{(m+j-1)} \cdot g^{(m-j)} \Big|_{t_i^+}^{t_{i+1}^-} + (-1)^m \int_{t_i}^{t_{i+1}} f^{(2m)} \cdot g \\
&= \sum_{i=1}^{n} \sum_{j=1}^{m} (-1)^j \left(\mathrm{jmp}_{t_i} f^{(m+j-1)}\right) \cdot g^{(m-j)}(t_i) \; + \; 0 \\
&= \sum_{i=1}^{n} \sum_{j=1}^{m} (-1)^{m-j+1} \left(\mathrm{jmp}_{t_i} f^{(2m-j)}\right) \cdot g^{(j-1)}(t_i) \\
&= \langle \Psi_t f, \Lambda_t g \rangle_Z .
\end{aligned}$$

With $g = f$,

$$J(f) = \langle D^m f, D^m f \rangle_Y = \langle \Psi_t f, \Lambda_t f \rangle_Z ,$$

proving (5.4). On passing to the adjoints,

$$\langle D^{m*} D^m f, g \rangle_X = \langle \Lambda_t^* \, \Psi_t f, g \rangle_X ,$$

and since this holds for all g in X, it follows that

$$D^{m*} D^m f = \Lambda_t^* \, \Psi_t f.$$

In particular, $D^{m*} D^m f$ is in the range of the map Λ_t^*. Since $t \in \Delta_n$ (i.e., there are no repetitions of the data sites), then Λ_t^* is 1-1 (by Proposition 3.2), and so $(\Lambda_t^*)^{-1}$ is well-defined on the range of Λ_t^*. Hence, (5.5) follows. □

The earlier results in this section assumed that the data sites had not repetitions, i.e., $t_i \neq t_{i+1}$ for all i. However, in the characterization stated next, repetitions are allowed. The main difficulty in this case is that the map $\Lambda_t : X \longrightarrow Z$ is not onto. To remedy this difficulty, we will apply the above results with respect to the maximal strictly increasing subsequence of t, defined as

$$t' := (t_i : t_i \neq t_{i-1}). \tag{5.6}$$

Then, the data map $\Lambda_{t'}$ maps X onto *its* range, and certain results above apply with respect to t' and $\Lambda_{t'}$. Corresponding to t', let

$$\begin{aligned} w'_{ij} &:= \sum_{t_k = t'_i} w_{kj} \qquad \text{and} \\ z'_{ij} &:= \begin{cases} \sum_{t_k=t'_i} w_{kj} z_{kj} / w'_{ij}, & \text{if } w'_{ij} \neq 0; \\ 0, & \text{otherwise,} \end{cases} \end{aligned} \tag{5.7}$$

for $i{=}1{:}n'$ and $j{=}1{:}m$ with $n' := \#t'$. With this setup, we can now state a finite-dimensional characterization for solutions to (A). In the case that $t \in \Delta_n$, simply remove the "primes" where they appear.

Theorem 5.8. *Let $t \in \Delta_n^-$, $z \in Z$ and $\varepsilon \in \mathrm{IR}_+^{m\times n}$, and let Ψ_t be the "jump-map" from (2.2). Assume that Condition 4.1 holds. Let $\eta \in \Lambda_t^{-1} B_\varepsilon^-(z)$.*

(i) If $\ker D^m \cap \Lambda_t^{-1} B_\varepsilon^-(z) = \emptyset$, then η solves (A) iff for some $w \in \mathrm{IR}^{m\times n}$

$$\begin{aligned} &(w'\Lambda_{t'} + \Psi_{t'})\,\eta = w'z', \\ &w \geq 0, \quad w\,(\Gamma_t(f) - \varepsilon^2) = 0. \end{aligned} \tag{5.9}$$

In this case $\eta \in \$_{2m,t'}$.

(ii) If $\ker D^m \cap \Lambda_t^{-1} B_\varepsilon^-(z) \neq \emptyset$, then η solves (A) iff $\eta \in \ker D^m$.

Proof: Part (ii) was proved in Theorem 4.2. It was also shown in this theorem that, when $\ker D^m \cap \Lambda_t^{-1} B_\varepsilon^-(z) = \emptyset$, η solves (A) iff

$$D^{m*} D^m \eta + \Lambda_t^* w(\Lambda_t \eta - z) = 0 \tag{5.10}$$

for some $w \geq 0$ with $w_{ij} = 0$ when $|\lambda_{ij}\eta - z_{ij}| < \varepsilon_{ij}$. Now,

$$\Lambda_t^*\, w(\Lambda_t\eta - z) \;=\; \sum_{i=1}^{n}\sum_{j=1}^{m} w_{ij}(\lambda_{ij}\eta - z_{ij})\cdot\lambda_{ij} \;=\; \sum_{i=1}^{n'}\sum_{j=1}^{m}\sum_{t_k=t'_i} w_{kj}(\lambda_{kj}\eta - z_{kj})\cdot\lambda_{kj},$$

while

$$\begin{aligned} \sum_{t_k=t'_i} w_{kj}(\lambda_{kj}\eta - z_{kj})\cdot\lambda_{kj} &= \sum_{t_k=t'_i} w_{kj}(\lambda'_{ij}\eta - z_{kj})\cdot\lambda'_{ij} \\ &= \Big(\sum_{t_k=t'_i} w_{kj}\Big)(\lambda'_{ij}\eta)\cdot\lambda'_{ij} - \Big(\sum_{t_k=t'_i} w_{kj} z_{kj}\Big)\cdot\lambda'_{ij} \\ &= w'_{ij}(\lambda'_{ij}\eta)\cdot\lambda'_{ij} - w'_{ij} z'_{ij}\cdot\lambda'_{ij} \\ &= w'_{ij}(\lambda'_{ij}\eta - z'_{ij})\cdot\lambda'_{ij}, \end{aligned}$$

and so

$$\Lambda_t^* \, w(\Lambda_t \eta - z) = \sum_{i=1}^{n'} \sum_{j=1}^{m} w'_{ij}(\lambda'_{ij}\eta - z'_{ij}) \cdot \lambda'_{ij} = \Lambda_{t'}^* w'(\Lambda_{t'}\eta - z'). \tag{5.11}$$

Hence, by (5.10)

$$D^{m*} D^m \eta + \Lambda_{t'}^* \, w'(\Lambda_{t'}\eta - z') = 0. \tag{5.12}$$

Since there are no repetitions of the data sites in t', it follows by Proposition 3.2 (with t' in place of t) that $\Lambda_{t'}$ maps X 1-1 onto *its* target. As a consequence, $\eta \in \$_{2m,t'}$ by Corollary 5.2 with t' in place of t, and $\Psi_{t'}\eta = (\Lambda_{t'}^*)^{-1} D^{m*} D^m \eta$ by Lemma 5.3. By (5.12), $D^{m*} D^m \eta$ is in the range of the 1-1 map $\Lambda_{t'}^*$, and so,

$$(\Lambda_{t'}^*)^{-1} D^{m*} D^m \eta + w'(\Lambda_{t'}\eta - z') = 0.$$

By (5.5), but with t' in place of t,

$$\Psi_{t'}\eta = (\Lambda_{t'}^*)^{-1} D^{m*} D^m \eta,$$

and so

$$\Psi_{t'}\eta + \, w'(\Lambda_{t'}\eta - z') = 0,$$

which is equivalent to the corresponding equation in (5.9). □

By (5.9),

$$\Psi_{t'}\eta = -w'(\Lambda_{t'}\eta - z') = -w(\Lambda_t \eta - z).$$

That is,

$$\operatorname{jmp}_{t'_i} \eta^{(2m-j)} = (-1)^{m+j} w'_{ij}(\lambda'_{ij}\eta - z'_{ij}) = (-1)^{m+j} \sum_{t_k = t_i} w_{kj}(\lambda_{kj}\eta - z_{kj}), \tag{5.13}$$

for i=1:n' and j=1:m. In particular, $\operatorname{jmp}_{t'_i} \eta^{(2m-j)} = 0$ when $w'_{ij} = 0$. As a consequence, η reduces to a "natural spline" when $w_{ij} = 0$ for $j > 1$ (which is necessarily the case when $\varepsilon_{ij} = \infty$ for $j > 1$).

6. Uniqueness of the solutions to (A)

In this section, we first prove the unique solvability of the linear system in Theorem 5.8 for certain *fixed* weights, and then, by independent means, we verify the stronger result that the solutions to problem (A) are unique under similar conditions on the weights. In the case of repeated data sites, we follow the convention in (5.6) and (5.7).

Proposition 6.1. *Let $t \in \Delta_n^-$ and $w \in \mathbb{R}_{\ge 0}^{m\times n}$. Let $V_{t'}$ be the basis for $\$_{2m,t'}$ dual to $\Lambda_{t'}$. Suppose that $\ker D^m \cap \ker w\Lambda_t$=$\{0\}$. Then, the quadratic form associated to the map $(w'\,\Lambda_{t'} + \Psi_{t'})V_{t'}$ is positive definite on $Z' := (\mathbb{R}^{m\times n'})^d$, and the restriction of $(w'\,\Lambda_{t'} + \Psi_{t'})$ to $\$_{2m,t'}$ is invertible.*

Proof: Let $\alpha' \in Z'$. Since $\Lambda_{t'}$ maps $\$_{2m,t'}$ onto Z', then there exists an $f \in \$_{2m,t'}$ such that $f = V_{t'}\,\alpha'$. For this f,

$$\Lambda_{t'} f = \Lambda_{t'} V_{t'}\,\alpha' = \alpha'.$$

Then,

$$\begin{aligned}
\alpha'^T(w'\,\Lambda_{t'} + \Psi_{t'})V_{t'}\,\alpha' &= \alpha'^T w'\,\Lambda_{t'}V_{t'}\,\alpha' + \alpha'^T\Psi_{t'}V_{t'}\,\alpha' \\
&= \alpha'^T w'\,\alpha' + \langle \Psi_{t'}V_{t'}\,\alpha', \alpha' \rangle_{Z'} \\
&= (\Lambda_{t'}f)^T w'\,(\Lambda_{t'}f) + \langle \Psi_{t'}f, \Lambda_{t'}f \rangle_{Z'} \\
&= (\sqrt{w'}\,\Lambda_{t'}f)^T(\sqrt{w'}\,\Lambda_{t'}f) + J(f),
\end{aligned}$$

the last equality by (5.4). Since $w \geq 0$, and hence $w' \geq 0$, the right hand side is non-negative. Moreover, if it is zero, then $f \in \ker J = \ker D^m$ and $f \in \ker \sqrt{w'}\,\Lambda_{t'} = \ker\, w'\,\Lambda_{t'}$. Since $\ker\, w'\,\Lambda_{t'} = \ker\, w\,\Lambda_t$, then $f = 0$ when $\ker D^m \cap \ker\, w\Lambda_t=\{0\}$.

Consequently, $(w'\,\Lambda_{t'} + \Psi_{t'})V_{t'}$ is positive definite on Z', and in particular, it is invertible. Since $V_{t'}$ is invertible as a map to $\$_{2m,t'}$, the restriction of $(w'\,\Lambda_{t'} + \Psi_{t'})$ to $\$_{2m,t'}$ is invertible. $\square$

By Proposition 6.1, there is only one solution to problem (A) that corresponds to each sequence of weights satisfying (5.9), when $\ker D^m \cap \ker\, w\Lambda_t=\{0\}$. Under certain additional conditions, uniqueness to (A) follows as well, as stated in part (iii) in the next result.

Proposition 6.2. *Let $t \in \Delta_n^-$, $z \in Z$ and $\varepsilon \in \mathbb{R}_+^{m\times n}$. Assume that Condition 4.1 holds. Assume also that $\ker D^m \cap \Lambda_t^{-1}B_\varepsilon^-(z)=\emptyset$. Let η and $\hat\eta$ be solutions to (A), and let w and $\hat w$ be as described in Theorem 5.8 for η and $\hat\eta$, respectively. Then,*

(i) $\lambda_{ij}\eta = \lambda_{ij}\hat\eta$ *if* $w_{ij} \neq 0$ *or* $\hat w_{ij} \neq 0$ *($\Longrightarrow$ η and $\hat\eta$ agree on active constraints).*

(ii) $w = \hat w$ *if, for each i and j, the sequence*

$$S_{ij} := (\lambda_{kj}\eta - z_{kj} : t_k = t_i \text{ and } |\lambda_{kj}\eta - z_{kj}| = \varepsilon_{kj})$$

is linearly independent (unique weights).

(iii) $\eta = \hat\eta$ *if* $\ker D^m \cap \ker\, w\Lambda_t=\{0\}$ *(uniqueness).*

Proof: We start by proving (i), specifically, by proving that both w_{ij} and $\hat w_{ij}$ must be zero when $\hat\lambda_{ij}\eta \neq \lambda_{ij}\eta$. So, suppose that $v := \lambda_{ij}\eta - \lambda_{ij}\hat\eta \neq 0$ for some i in $\{1{:}n\}$ and j in $\{1{:}m\}$. By Theorem 5.8, $\hat w_{kj} \geq 0$ and $w_{kj} \geq 0$ for all k such that $t_k = t_i$. Moreover, if, for example, $w_{kj} > 0$, then $|\lambda_{kj}\eta - z_{kj}| = \varepsilon_{kj}$, hence, $\lambda_{kj}\eta - z_{kj}$ is normal to the supporting hyperplane to $B_{\varepsilon_{kj}}^-(z_{kj})$ at $\lambda_{kj}\eta$ and $w_{kj}(\lambda_{kj}\eta - z_{kj}) \cdot v > 0$, while $w_{kj}(\lambda_{kj}\eta - z_{kj}) \cdot v \geq 0$ always holds, with equality only if $w_{kj} = 0$. Therefore,

$$\sum_{t_k=t_i} w_{kj}(\lambda_{ij}\eta - z_{kj}) \cdot v \geq 0 \tag{6.3}$$

with strict inequality iff $w_{kj} > 0$ for some k such that $t_k = t_i$. Symmetrically,

$$\sum_{t_k=t_i} \hat w_{kj}(\lambda_{ij}\hat\eta - z_{kj}) \cdot (-v) \geq 0 \tag{6.4}$$

with strict inequality iff $\hat w_{kj} > 0$ for some k such that $t_k = t_i$.

To complete the proof of (i), note by Theorem 3.1 that $\hat\eta-\eta$ is in $\ker D^m$. Hence, $\mathrm{jmp}_{t_i}(\hat\eta^{(2m-j)}-\eta^{(2m-j)})=0$ for $i{=}1{:}n$ and $j{=}1{:}m$, and by (5.13)

$$\sum_{t_k=t_i}\hat w_{kj}(\lambda_{ij}\hat\eta-z_{kj})=\sum_{t_k=t_i}w_{kj}(\lambda_{ij}\eta-z_{kj}). \tag{6.5}$$

By (6.3) and (6.4), this implies that

$$0\ge\sum_{t_k=t_i}\hat w_{kj}(\lambda_{ij}\hat\eta-z_{kj})\cdot v=\sum_{t_k=t_i}w_{kj}(\lambda_{ij}\eta-z_{kj})\cdot v\ge 0,$$

which can only occur with equality in these inequalities, and moreover, iff $\hat w_{kj}=w_{kj}=0$ for all k such that $t_k=t_i$. This completes the proof of (i).

To verify (ii), we first note by (i) that $\hat w_{ij}=w_{ij}=0$ when $\lambda_{ij}\hat\eta\ne\lambda_{ij}\eta$. Hence, it remains to consider the case that $\lambda_{ij}\hat\eta=\lambda_{ij}\eta$. Assuming this, it follows by (6.5) that

$$\sum_{t_k=t_i}(\hat w_{kj}-w_{kj})(\lambda_{ij}\eta-z_{kj})=0. \tag{6.6}$$

When $|\lambda_{ij}\eta-z_{kj}|<\varepsilon_{kj}$, then $w_{kj}=0$, and moreover $\hat w_{kj}=0$ since either $|\lambda_{ij}\hat\eta-z_{kj}|<\varepsilon_{kj}$ or $\lambda_{ij}\hat\eta\ne\lambda_{ij}\eta$ (applying part (i) here). Hence, (6.6) is equivalent to

$$\sum_{\lambda_{kj}\eta-z_{kj}\in S_{ij}}(\hat w_{kj}-w_{kj})(\lambda_{ij}\eta-z_{kj})=0,$$

which implies that $\hat w_{kj}=w_{kj}$ for all k such that $t_k=t_i$ when the sequence S_{ij} is linearly independent, as assumed (and as is trivially the case when $t\in\Delta_n$). This proves (ii).

Finally, since, by (i), $\lambda_{ij}\hat\eta=\lambda_{ij}\eta$ when $w_{ij}\ne 0$, it follows that $w\Lambda_t\hat\eta=w\Lambda_t\eta$. Therefore, $\hat\eta-\eta$ is in $\ker w\Lambda_t$, and so $\hat\eta=\eta$ when $\ker D^m\cap\ker w\Lambda_t{=}\{0\}$, proving (iii). □

Part (i) of Proposition 6.2 states that distinct minimizers have the same active constraints when $\ker D^m\cap\Lambda_t^{-1}B_\varepsilon^-(z){=}\emptyset$, and, moreover, the same function values at these constraints. Hence, minimizers can differ only at inactive constraints. However, even when $\ker D^m\cap\Lambda_t^{-1}B_\varepsilon^-(z){=}\emptyset$, there may be more than one solution to (A), as in the following example.

Example 6.7. *Let $n{=}\ m{=}\ 2$ and $d=1$. Let $z_{11}=z_{21}=1$, $\varepsilon_{11}=\varepsilon_{21}=1$, $z_{12}=1$, $z_{22}=-1$ and $\varepsilon_{12}=\varepsilon_{22}=1/4$. Then $\ker D^m\cap\Lambda_t^{-1}B_\varepsilon^-(z){=}\emptyset$, but the solutions to problem (A) are not unique.*

Proof: Since there are feasible functions, then solutions exist by Theorem 3.1. For the given configuration, $B^-_{\varepsilon_{12}}(z_{12})\cap B^-_{\varepsilon_{22}}(z_{22})=\emptyset$, and so the end slopes of the feasible functions must differ. Since the polynomials in $\ker D^m$ are linear, then necessarily $\ker D^m\cap\Lambda_t^{-1}B_\varepsilon^-(z){=}\emptyset$.

Let η be one such solution. If $\eta(1)\ne\eta(0)$, then $\eta(1-\cdot)$ is a solution since it satisfies the constraints and $J(\eta(1-\cdot))=J(\eta)$. On the other hand, if $\eta(1)=\eta(0)$, then either $1+\eta$ or $-1+\eta$ is a solution. □

Although non-uniqueness in (A) may occur, solutions generally are unique for small m. Hence, it is perhaps not so important to identify all those configurations of the data (z, ε, t) that lead to uniqueness, and is moreover a tricky matter since the Hermite-type constraints often reduce to "Birkhoff" constraints when, for example, $w_{ij} \neq 0$ but $w_{i,j-1} = 0$ for some i and j. However, a partial attempt in this direction was made in [K99a]. Two special cases where uniqueness does hold are when $m = 2$ and there is no polynomial of degree $2m-1$ that meets the constraints, and when $w_{ij} = \infty$ for $j > 1$ and $\ker D^m \cap \Lambda_t^{-1} B_\varepsilon^-(z) = \emptyset$. For the second case, which was already proved in [L69] when $d = 1$, it follows that $w_{i1} \neq 0$ for at least m weights, in which case $\ker D^m \cap \ker w\Lambda_t = \{0\}$, and uniqueness follows by Proposition 6.2.

7. A necessary optimality condition for the solutions to (B)

In this section we derive a first-order necessary optimality condition for the (local) solutions (η, t) to (B). Since, for such a solution, η necessarily solves (A) for these *fixed* t, it follows by Theorem 5.8 that η satisfies (5.9) and $\eta \in \$_{2m,t'}$. Hence, the solutions to (B) are splines curves.

To obtain a necessary condition, we first consider those functions in X that are splines with data sites $t \in \Delta_n$, i.e., data sites with no repetitions. For this, let

$$\$_{2m} := \{f \in X : f \in \$_{2m,t} \text{ for some } t \in \Delta_n\}.$$

To parametrize $\$_{2m}$, let

$$\varphi : Z \times \Delta_n \longrightarrow \$_{2m} : (\alpha, t) \longrightarrow V_t\, \alpha = \sum_{ij} \alpha_{ij}\, v_{ij}$$

with $V_t = [v_{ij}]$ the basis-map for $\$_{2m,t}$ that is *dual* to Λ_t; the "piecewise Hermite" basis. In particular,

$$\Lambda_t f = \Lambda_t \varphi(\alpha, t) = \Lambda_t V_t\, \alpha = \alpha$$

when $f = V_t\, \alpha$. As a consequence, the constraints $|\lambda_{ij} f - z_{ij}| \leq \varepsilon_{ij}$ conveniently reduce to $|\alpha_{ij} - z_{ij}| \leq \varepsilon_{ij}$ when $f = V_t\, \alpha$, and problem (A) simplifies to

$$\text{(7.1)} \qquad \underset{\alpha \in B_\varepsilon^-(z),\ t \in \Delta_n}{\text{minimize}} \quad J \circ \varphi(\alpha, t).$$

The necessary condition derived here is obtained by taking variations with respect to the coefficients α and the data sites t, separately. Since the case of fixed t was considered in problem (B), it remains to consider variations of t with α fixed. This turns out to be particularly convenient in the setup here since the data sites t can be varied freely in Δ_n without affecting the constraint $\alpha \in B_\varepsilon^-(z)$ in (7.1). Hence, it remains to consider the unconstrained minimization problem

$$\text{(7.2)} \qquad \underset{t \in \Delta_n}{\text{minimize}}\ J \circ \varphi\,(\alpha, t)$$

for fixed $\alpha \in B_\varepsilon^-(z)$.

To obtain an optimality condition for local solutions, we need to find stationary points of (7.2). For this, we differentiate $J \circ \varphi$ with respect to t_i for i=2:n−1 (with $t_1 = 0$ and $t_n = 1$ fixed). For this, let ∂_{t_i} and $\partial_{t_i^\pm}$ denote partial derivative operators. For example, at $s \in [0\,.\,.1]$,

$$[\partial_{t_i^+}\varphi(\alpha,t)](s) := \lim_{\epsilon\downarrow 0}\frac{\varphi(\alpha,t+\epsilon e_i)(s)-\varphi(\alpha,t)(s)}{\epsilon}$$

with $e_i := (\overbrace{0,\ldots,0}^{i-1},1,0,\ldots,0) \in \mathbb{R}^n$. Note that since $t_i < t_{i+1}$ for all i, then $t+\epsilon e_i \in \Delta_n$ for small enough ϵ. To simplify notation, let $\partial_{t_i^\pm} f := \partial_{t_i^\pm}\varphi(\alpha,t)$ when $f = \varphi(\alpha,t)$.

Lemma 7.3. *Let $f := \varphi(\alpha,t)$ for $(\alpha,t) \in Z \times \Delta_n$. For i=2:n−1 and j=1:m,*

$$[\partial_{t_i^\pm} f^{(j-1)}](t_k) = \begin{cases} -f^{(j)}(t_k^\pm), & \text{if } k = i; \\ 0, & \text{otherwise.}\end{cases}$$

For $j < m$, "±" can be removed.

Proof: With α fixed,

$$\Lambda_{t+\epsilon\, e_i}\varphi(\alpha,t+\epsilon\, e_i) = \alpha,$$

and since $(t+\epsilon\, e_i)(k) = t_k$ when $k \neq i$, it follows that

$$D^{j-1}\varphi(\alpha,t+\epsilon\, e_i)(t_k) = D^{j-1}\varphi(\alpha,t+\epsilon\, e_i)((t+\epsilon\, e_i)(k)) = \alpha_{ij}$$

when $k \neq i$. In this case,

$$[\partial_{t_i^+} f^{(j-1)}](t_k) = [\partial_{t_i^+} D^{j-1}\varphi(\alpha,t)](t_k) = \lim_{\epsilon\downarrow 0}\frac{\alpha_{ij}-\alpha_{ij}}{\epsilon} = 0.$$

Likewise, $[\partial_{t_i^-} f^{(j-1)}](t_k) = 0$ when $k \neq i$.

Consider the case that $k = i$. Let

(7.4) $$p_i := p_i(t,\cdot) = \sum_{l=1}^{2m}\beta_l(t)(\cdot - t_i)^{l-1}/(l-1)!$$

with $\beta_l(t) = f^{(l-1)}(t_i^+)$, the Taylor polynomial representation for f on $(t_i\,.\,.\,t_{i+1})$. Then,

$$\partial_{t_i} p_i^{(j-1)} = \sum_{l=j}^{2m}(\partial_{t_i}\beta_l)(t)(\cdot - t_i)^{l-j}/(l-j)! - \sum_{l=j+1}^{2m}\beta_l(t)(\cdot - t_i)^{l-j-1}/(l-j-1)!,$$

and so

$$[\partial_{t_i} p_i^{(j-1)}](t_i) = (\partial_{t_i}\beta_j)(t) - \beta_{j+1}(t).$$

Now, $\beta_{m+1}(t),\ldots,\beta_{2m}(t)$ will vary as t_i varies, however, $\beta_j(t) = \alpha_{ij}$ for j=1:m, which are fixed independent of t_i. As a consequence,

$$[\partial_{t_i} p_i^{(j-1)}](t_i) = -\beta_{j+1}(t) = -p_i^{(j)}(t_i)$$

for j=1:m, implying that

$$[\partial_{t_i^+} f^{(j-1)}](t_i) = -f^{(j)}(t_i^+).$$

Similarly, it can be shown that

$$[\partial_{t_i^-} f^{(j-1)}](t_i) = -f^{(j)}(t_i^-)$$

on considering the restriction of f to $(t_{i-1}\,.\,.\,t_i]$. □

We will now determine the derivative of the map

$$J \circ \varphi : Z \times \Delta_n \longrightarrow \mathbb{R} : (\alpha, t) \longmapsto \int_0^1 |D^m f(s)|^2 \, ds$$

with respect to t_i for fixed α. For convenience, let $\partial_{t_i} J(f)$ denote $\partial_{t_i} J(\varphi(\alpha,t))$ with $f := \varphi(\alpha,t)$.

Proposition 7.5. *Let $f := \varphi(\alpha,t)$ for $(\alpha,t) \in Z \times \Delta_n$. For i=2:$n-1$,*

$$\partial_{t_i} J(f) = 2 \sum_{j=1}^{m} (-1)^{m+j} \, (\mathrm{jmp}_{t_i} f^{(2m-j)}) \cdot f^{(j)}(t_i),$$

with $f^{(m)}(t_i) := (f^{(m)}(t_i^+) + f^{(m)}(t_i^-))/2$.

Proof: First, note that

$$\partial_{t_i} J(f) = \sum_{k=1}^{n-1} \partial_{t_i} \int_{t_k}^{t_{k+1}} f^{(m)}(s) \cdot f^{(m)}(s) \; ds, \tag{7.6}$$

and that the restriction of f to the interval $(t_i \,.\,.\, t_{i+1})$ is equivalent to the Taylor polynomial p_i defined in (7.4). For each i, the functions β_l in (7.4) are rational functions of the differences $t_{i\pm1} - t_i$, which are bounded away from zero when $t \in \Delta_n$, as assumed here. Therefore, the map

$$(t,s) \longmapsto p_i^{(j-1)}(t,s)$$

is continuously differentiable (for all j). As a consequence, Leibniz' rule applies to (7.6), i.e.,

$$\partial_{t_i} J(f) = f^{(m)} \cdot f^{(m)} \Big|_{t_i^+}^{t_i^-} \; + \; 2 \sum_{k=1}^{n-1} \int_{t_k}^{t_{k+1}} f^{(m)} \cdot \partial_{t_i} f^{(m)}, \tag{7.7}$$

and the operators ∂_{t_i} and D^j commute. By integration by parts, and with $f^{(2m)} \equiv 0$, it follows that

$$\begin{aligned} \int_{t_k}^{t_{k+1}} f^{(m)} \cdot \partial_{t_i} f^{(m)} &= \int_{t_k}^{t_{k+1}} f^{(m)} \cdot D^m \partial_{t_i} f \\ &= 2 \sum_{j=1}^{m} (-1)^{m+j} \, f^{(2m-j)} \cdot D^{j-1} \partial_{t_i} f \Big|_{t_k}^{t_{k+1}} \\ &= 2 \sum_{j=1}^{m} (-1)^{m+j} \, f^{(2m-j)} \cdot \partial_{t_i} f^{(j-1)} \Big|_{t_k}^{t_{k+1}}. \end{aligned} \tag{7.8}$$

By Lemma 7.3 $[\partial_{t_i^\pm} f^{(j-1)}](t_k)$ equals $-f^{(j)}(t_i^\pm)$ when $k = i$ and is 0 otherwise, hence, with (7.8), (7.7) reduces to

$$\begin{aligned} \partial_{t_i} J(f) &= f^{(m)} \cdot f^{(m)} \Big|_{t_i^+}^{t_i^-} \; + \; 2 \sum_{j=1}^{m} (-1)^{m+j} \, f^{(2m-j)} \cdot f^{(j)} \Big|_{t_i^-}^{t_i^+} \\ &= (\mathrm{jmp}_{t_i} f^{(m)}) \cdot (f^{(m)}(t_i^+) + f^{(m)}(t_i^-)) \; + \; 2 \sum_{j=1}^{m-1} (-1)^{m+j} \, (\mathrm{jmp}_{t_i} f^{(2m-j)}) \cdot f^{(j)}(t_i)\,, \\ &= 2 \sum_{j=1}^{m} (-1)^{m+j} \, (\mathrm{jmp}_{t_i} f^{(2m-j)}) \cdot f^{(j)}(t_i) \end{aligned}$$

with $f^{(m)}(t_i) = (f^{(m)}(t_i^+) + f^{(m)}(t_i^-))/2$. $\square$

A necessary condition for (local) solutions (η, t) to problem (B) is stated next. To handle repeated data sites in the sequence t, Proposition 7.5 will be applied with respect to the sequence t' in (5.6). Also let $n' := \#t'$ and w', z' and ε' as in (5.7), and let $\lambda_{ij}^{\pm}$ be as defined in (2.2).

Theorem 7.9. *Let $z \in Z$ and $\varepsilon \in \mathrm{IR}_{+}^{m\times n}$. Suppose that (η, t) is a local solution to problem (B). Assume that Condition 4.1 holds with respect to t, and that $\ker D^m \cap \Lambda_t^{-1} B_{\varepsilon}^{-}(z) = \emptyset$. Then $\eta \in \mathrm{ran}(V_{t'})$ with $V_{t'}$ the basis for $\$_{2m,t'}$ that is dual to $\Lambda_{t'}$, and for some $w \in \mathrm{IR}^{m\times n}$,*

$$
\begin{aligned}
&(w'\Lambda_{t'} + \Psi_{t'})\,\eta = w'z', \\
&w \geq 0, \quad w\,(\Gamma_t(f) - \varepsilon^2) = 0, \\
&\sum_{j=1}^{m} w'_{ij}(\lambda'_{ij}\eta - z'_{ij}) \cdot \lambda'_{i,j+1}\eta = 0 \quad \text{for } i{=}2{:}n'{-}1,
\end{aligned}
\tag{7.10}
$$

with $\lambda_{i,m+1} = (\lambda_{i,m+1}^{+} + \lambda_{i,m+1}^{-})/2$.

Proof: Since η necessarily solves problem (A) for the fixed t, then $\eta \in \$_{2m,t'}$ and the first two equations in (7.10) follow by Theorem 5.8 part (i). Since t' is a local minimizer of $J \circ \varphi(\alpha', \cdot)$ for fixed $\alpha' \in Z'$ such that $\eta = V_{t'}\alpha'$, then $\partial_{t'_i} J(\eta) = 0$. Therefore,

$$\partial_{t'_i} J(\eta) = 2 \sum_{j=1}^{m} (-1)^{m+j}\,(\mathrm{jmp}_{t'_i}\eta^{(2m-j)}) \cdot \eta^{(j)}(t'_i) = 0$$

by Proposition 7.5 with t', $\Delta_{n'}$, $\$_{2m,t'}$ and $V_{t'}$ in place of t, Δ_n, $\$_{2m,t}$ and V_t, respectively, and with $\eta^{(m)}(t'_i) := (\eta^{(m)}((t'_i)^+) + \eta^{(m)}((t'_i)^-))/2$. By (5.13)

$$\mathrm{jmp}_{t'_i}\eta^{(2m-j)} = (-1)^{m+j} w'_{ij}(\lambda'_{ij}\eta - z'_{ij}),$$

and the third equation in (7.10) follows. □

Note that, on expanding out w'_{ij}, λ'_{ij} and z'_{ij}, the third equation in (7.10) is equivalent to

$$\sum_{t_k = t'_i} \sum_{j=1}^{m} w_{kj}(\lambda_{kj}\eta - z_{kj}) \cdot \lambda_{k,j+1}\eta = 0,$$

for each $i{=}2{:}n'{-}1$. This is an "orthogonality" condition. Indeed, assuming that $t \in \Delta_n$ and $m > 1$, this equations reduces to

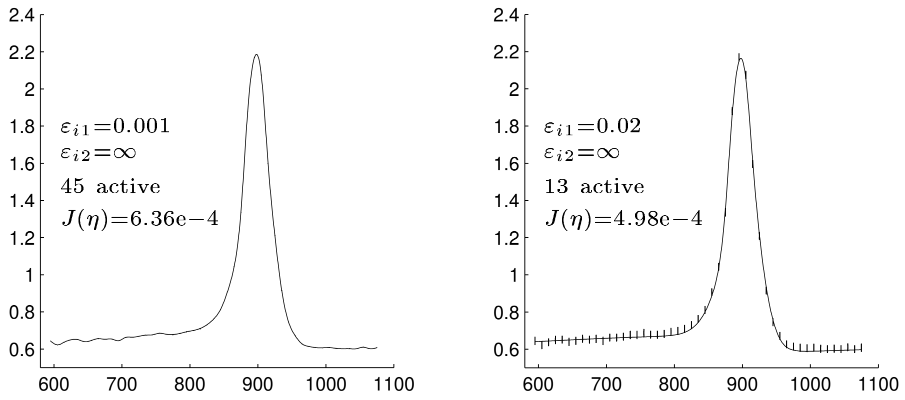
$$(\eta(t_i) - z_{i1}) \cdot \eta'(t_i) = 0$$

at t_i when $w_{i1} > 1$ and $w_{ij} = 0$ for all $j > 1$. In particular, this occurs for "natural" spline curves.

Theorem 7.9 was derived, in part, by taking variations of the data sites in directions that maintain their multiplicities, while holding the coefficients α fixed. This prevents difficulties that can occur when data sites are separated along a variation. However, it is shown in [K99b] that sequences $((\eta^l, t^l))$ converge under certain conditions when $t^l \longrightarrow t$ and when η^l solves problem (A) for fixed t^l, even when there are repetitions. This contrasts spline "interpolation" with free data sites where the functional J may become unbounded on similar sequences.

8. Examples

In the examples that follow $m = 2$, and consequently the curves are cubic splines. In Figure 8.1, two near-interpolating "functions" are fit to the titanium heat data in [dB78: page 226], with the abscissae of the data re-scaled over $[0\,..1]$ to conform to the setup here. In (a) the tolerances are small, and consequently the curve mirrors the inflections (possibly errors) in the data. With the larger tolerances in (b) (as indicated by the "gates"), these errors are smoothed over, and a smoother curve results. Moreover, of the 49 data points, 45 are active in (a) but only 13 in (b). This means that the curve in (a) needs about 45 polynomial pieces, while the curve in (b) needs only about 13; a significant reduction. Hence, near-interpolation provides an automatic mechanism for choosing optimal data sites (hence knots) in spline curves that is generally less than the size of the data set.



(a) (b)

Figure 8.1. Titanium heat data: 49 data points, $m = 2$, $d = 1$, solves (A).

As with the data in Figure 8.1, the data in 8.2 appears to have some error. Consequently, the curve fit in (a) is rather unwieldy. To better recover the underlying "shape", larger tolerances are introduced (displayed as circles), producing the curve in (b), which moreover has less "energy", as measured by J.

(a) ε_{i1}=0.01 (b) ε_{i1}=0.1

Figure 8.2. Shepherd's crook: $m = 2$, $d = 2$, $\varepsilon_{i2} = \infty$, solves (B).

In Figure 8.3, a sharp corner is approximated by near-interpolants to problem (A) for prescribed data sites t. For (a), the tolerances ε_{i2} are infinite for all i, and for (b) these tolerances are chosen small at the "corners". Consequently, the curve in (a) is a natural spline, unlike that in (b). At each corner there is a horizontal tangent $(1, 0)$ and a vertical tangent $(0, -1)$ prescribed. The curvature of the curves at these corners is moreover controlled by the tolerances ε_{i1}, i.e., the radii of the displayed circles. A blowup of one of the corners in (b) is displayed in (c), with the $*$'s at the points $\eta(t_i)$.

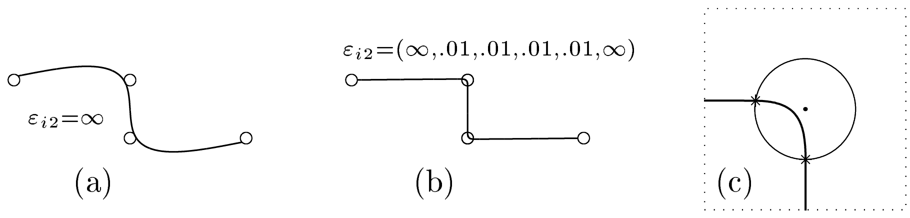


Figure 8.3. "Sharp" corners: $m = 2$, $d = 2$, $\varepsilon_{i1} = 0.05$, solves (A).

In Figure 8.4 the solution to problem (A) for two common choices of parametrizations are compared to the solution to problem (B). As a consequence of the freedom to select an optimal parametrization, there are more feasible curves to choose from in (B), and consequently, the third curve has less energy than the first two, as measured by J. In general, parametrizations can have a significant effect on the resulting curves.

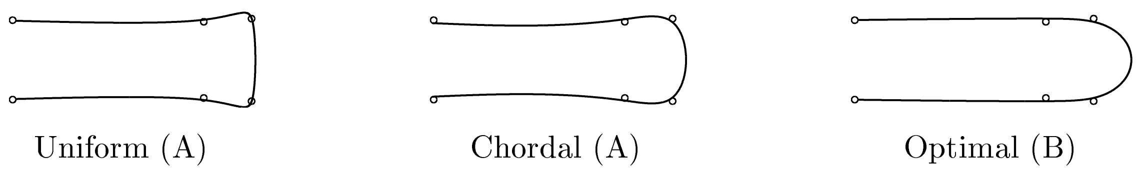


Figure 8.4. Various parametrizations: fixed and free data sites, $m = 2$, $d = 2$, $\varepsilon_{i2} = 0$.

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