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A General Method for the Construction of Interpolating or Smoothing Spline-Functions

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I. Introduction

Many authors have been studying spline-functions the past few years (see bibliography, non-exhaustive, at the end). The effective use of spline-functions poses some numerical problems: certain methods turned out to be unstable and completely impractical, even in simple cases.

First we consider the most elementary example of a spline-function:

Let $H^q = H^q[a, b]$ be the Hilbert space of real functions with absolutely continuous $(q-1)^{\text{st}}$ and square integrable q^{th} derivative with the inner product:

$$(f, g)_q = \sum_{j=0}^{q} \int_a^b f^{(j)}(t) \cdot g^{(j)}(t)\, dt, \qquad \left(\|f\|_q = (f, f)_q^{\frac{1}{2}}\right) \tag{1.1}$$

and let $H^0 = H^0[a, b]$ be the space of square integrable functions with the usual inner product:

$$(f, g)_0 = \int_a^b f(t) \cdot g(t)\, dt, \qquad \left(\|f\|_0 = (f, f)_0^{\frac{1}{2}}\right). \tag{1.2}$$

We define $\Phi \subset H^q$ by:

$$\Phi = \{f \in H^q : f(x_i) = r_i,\ i = 1, \ldots, n\} \tag{1.3}$$

where the $x_i \in [a, b]$ $(x_i < x_{i+1})$ and the $r_i \in R$ are prescribed. We know that the element $\sigma \in \Phi$ (called a spline-function) satisfying:

$$\|\sigma^{(q)}\|_0 = \min_{f \in \Phi} \|f^{(q)}\|_0 \tag{1.4}$$

exists and is unique (if $n \geq q$). It is composed of pieces of polynomials of degree $2q-1$ which agree at the x_i up to the $(2q-2)^{\text{nd}}$ derivative (included), and satisfies:

$$\begin{aligned} \sigma^{(j)}(a) = \sigma^{(j)}(b) = 0, &\qquad j = q, q+1, \ldots, 2q-2, \\ \sigma^{(2q-1)}(x) \equiv 0, &\qquad \text{all} \quad x \notin [x_1, x_n]. \end{aligned} \tag{1.5}$$

Therefore, we can write:

$$\sigma(x) = a_0 + a_1 x + \cdots + a_{q-1} x^{q-1} + \sum_{i=1}^{n} \lambda_i (x - x_i)_+^{2q-1} \tag{1.6}$$

with

$$(E)_+ = \begin{cases} E & \text{if } E \geq 0, \\ 0 & \text{if } E < 0. \end{cases}$$

It is practically impossible to obtain the coefficients a_i and λ_i with a good accuracy by direct resolution (see CARASSO [17]) when n or q is large (for example $q \geqq 3$ or $n \geqq 30$). Even if the λ_i and a_i have been determined accurately, the form (1.6) implies loss of accuracy (by subtraction of neighboring numbers) and $\sigma(x)$ computed by (1.6) no longer satisfies the interpolation equations (1.3).

We propose here a general method, based on the properties of orthogonality of the spline functions. This method has proved to be stable even for a large number of functionals (see CARASSO [17—19]). We consider the abstract spline-functions in a Hilbert space, as introduced by ATTEIA [9, 10, 12].

We shall give three examples of applications treating in parallel the interpolating spline-functions and the smoothing spline-functions. ALGOL procedures corresponding to the most usual spline-functions can be obtained by writing to the second author.

The proposed method, as particularized in the example given above, is related to a method proposed by GREVILLE [30] using divided differences.

II. General Interpolating Spline-functions

The functionals:

$$f \in H^q[a, b] \to f(x_i) \in R$$

are linear and continuous ($q \geqq 1$). Hence, there exist unique $k_i \in H^q$ such that:

$$(k_i, f)_q = f(x_i), \qquad i = 1, \dots, n.$$

Let D^q be the continuous linear operator on H^q onto H^0 defined by $D^q f = f^{(q)}$. The spline-function σ is the element of H^q which minimizes $\|D^q \sigma\|_0$ satisfying

$$(k_i, \sigma)_q = r_i, \qquad i = 1, \dots, n.$$

We shall study the problem of the characterization and the construction of the spline-function in the more general framework introduced by ATTEIA. Let X and Y be real Hilbert spaces[1] (which generalize H^q and H^0 respectively) and $T \in \mathscr{L}[X, Y]$, the space of continuous linear operators on X into Y (T generalizes the operator D^q).

Consider n linearly independent elements $k_1, k_2, \dots, k_n$ in X, which span a (closed) subspace K. As usual, let $K^\perp$ be the (closed) orthogonal complement of K.

We denote:

$$r = [r_1, \dots, r_n] \in E = R^n \quad \text{(Euclidean space of dimension } n\text{)},$$

$$K_r^\perp = \{x \in X\colon\ (k_i, x)_X = r_i,\ i = 1, \dots, n\}. \tag{2.1}$$

Since:

$$K_r^\perp = x_r + K^\perp, \qquad \forall\, x_r \in K_r^\perp,$$

$K_r^\perp$ is a translate of the subspace $K^\perp$ and is closed. The set $K_r^\perp$ acts as the set Φ defined at (1.3).

We shall call an *interpolating spline function* (relative to T, $\{k_1 \dots k_n\}$ and r) any element $\sigma \in K_r^\perp$ which satisfies:

$$\|T\sigma\|_Y = \min_{x \in K_r^\perp} \|Tx\|_Y. \tag{2.2}$$

[1] The same study can easily be transposed into the case of complex Hilbert space

If $f = T\sigma$, then:

(2.3) $$\|f\|_Y = \min_{y \in TK_r^\perp} \|y\|_Y.$$

Since:

(2.4) $$TK_r^\perp = y_r + TK^\perp, \quad \forall y_r \in TK_r^\perp$$

$TK_r^\perp$ is a translate of the subspace $TK^\perp$. It is clear that $TK_r^\perp$ is closed iff $TK^\perp$ is closed. Let $\mathcal{N}(T)$ denote the kernel (null space) of T.

Proposition 2.1. *If $TK^\perp$ is closed and $\mathcal{N}(T) \cap K^\perp = \{\theta_X\}$ then, for each $r \in E$, there exists a unique spline-function σ satisfying (2.2) which is determined by the conditions:*

(2.5) $$\sigma \in K_r^\perp,$$

(2.6) $$f = T\sigma \in (TK^\perp)^\perp.$$

Proof. Since $TK_r^\perp$ is closed, there exists a unique $f \in TK_r^\perp$ at minimum distance of the origin θ_Y. It is the orthogonal projection of θ_Y on $TK_r^\perp$. We have: f orthogonal to $TK^\perp$ and $f \in TK_r^\perp$.

Now, since $\mathcal{N}(T) \cap K^\perp = \{\theta_X\}$, T is one-to-one on $K^\perp$ and $K_r^\perp$: there exists a unique σ in $K_r^\perp$ such that $T\sigma = f$. q.e.d.

It will be shown that $TK^\perp$ is closed whenever $\mathcal{N}(T) \cap K^\perp = \{\theta_X\}$ and the range $\mathcal{R}(T)$ is closed.

The determination of f and σ will be reduced to the solution of a certain finite algebraic system. For these purposes some general properties of adjoint and projection operators are needed.

III. Operators and Adjoints

For each $T \in \mathcal{L}[X, Y]$, the adjoint operator $T^* \in \mathcal{L}[Y, X]$ is defined by:

(3.1) $$(Tx, y)_Y = (x, T^*y)_X.$$

It follows that $T^{**} = T$ and

(3.2) $$\begin{aligned} \mathcal{R}(T)^\perp &= \mathcal{N}(T^*); & \mathcal{R}(T^*)^\perp &= \mathcal{N}(T); \\ \overline{\mathcal{R}(T)} &= \mathcal{N}(T^*)^\perp & \overline{\mathcal{R}(T^*)} &= \mathcal{N}(T)^\perp. \end{aligned}$$

We recall the closed-range theorem (YOSIDA [58], p. 205):

(3.3) $\mathcal{R}(T)$ *is closed iff* $\mathcal{R}(T^*)$ *is closed.*

Let M be any subspace of X. By (3.1), $y \in (TM)^\perp$ iff $T^*y \in M^\perp$, which generalizes $\mathcal{R}(T)^\perp = \mathcal{N}(T^*)$. Hence,

(3.4) $$(TM)^\perp = (T^*)^{\sim 1} M^\perp,$$

where $(T^*)^{\sim 1}$ is the set function inverse,

(3.5) $$\overline{TM} = [(T^*)^{\sim 1} M^\perp]^\perp,$$

(3.6) $$T^*(TM)^\perp = \mathcal{R}(T^*) \cap M^\perp.$$

Further identities are obtained if M is replaced by $M^\perp$ or T by T^*.

IV. Subspaces and Projections

Let K be any closed subspace of X (not necessarily finite dimensional as in § II). Let Q and P be the orthogonal (self-adjoint) projections onto K and $K^\perp$:

$$\mathscr{R}(Q) = K = \mathscr{N}(P) \qquad (4.1)$$
$$\mathscr{N}(Q) = K^\perp = \mathscr{R}(P).$$

Defining $J \in \mathscr{L}[K^\perp, X]$ by

$$J x = x, \quad \forall x \in K^\perp, \qquad (4.2)$$

then (3.1) yields:

$$J^* = P. \qquad (4.3)$$

Let T_M denote the restriction of an operator T to a subspace M. Then:

$$T_{K^\perp} = T J, \qquad (4.4)$$

$$T_{K^\perp}{}^* = J^* T^* = P T^*, \qquad (4.5)$$

$$\mathscr{R}(T_{K^\perp}) = T K^\perp, \qquad (4.6)$$

$$\mathscr{R}(T_{K^\perp}{}^*) = P \mathscr{R}(T^*). \qquad (4.7)$$

V. Relations between Subspaces

Again let $\dim(K) = n$ with basis $\{k_1, \ldots, k_n\}$. Define $A \in \mathscr{L}[X, E]$ by:

$$A(x) = [(k_1, x), \ldots, (k_n, x)], \quad \forall x \in X. \qquad (5.1)$$

We have:

$$K_r^\perp = \{x \in X \colon A x = r\}. \qquad (5.2)$$

By (3.1), $A^* \in \mathscr{L}[E, X]$ has the form:

$$A^* y = \sum_{i=1}^{n} y_i k_i, \quad \forall y = [y_1, \ldots, y_n] \in E. \qquad (5.3)$$

Note that:

$$\mathscr{N}(A) = K^\perp = \mathscr{R}(A^*)^\perp; \qquad \mathscr{N}(A)^\perp = K = \mathscr{R}(A^*) \qquad (5.4)$$
$$\mathscr{R}(A) = E = \mathscr{N}(A^*)^\perp; \qquad \mathscr{R}(A)^\perp = \{\theta_E\} = \mathscr{N}(A^*),$$

$$\exists (A^*)^{-1} \in \mathscr{L}[K, E]. \qquad (5.5)$$

Let N be an arbitrary subspace of X. The case $N = \mathscr{N}(T)$ will be of primary interest. Assume

$$N \cap K^\perp = \{\theta_X\}. \qquad (5.6)$$

Then $N \cap \mathscr{N}(A) = \{\theta_X\}$, so A maps N one-to-one into E: Therefore

$$\exists A_N^{-1} \in \mathscr{L}[A N, N], \qquad (5.7)$$

$$\dim(N) \leq n. \qquad (5.8)$$

Proposition 5.1. *If* $\dim(K) = n$, $\dim(N) = q$ *and* $N \cap K^\perp = \{\theta_X\}$, *then*

$$\dim(K \cap N^\perp) = n - q.$$

Proof. By (5.4) and (3.6):

$$K \cap N^{\perp} = \mathscr{R}(A^*) \cap N^{\perp} = A^*(AN)^{\perp}. \tag{5.9}$$

By (5.7), $\dim(AN) = \dim(N) = q$ and $\dim((AN)^{\perp}) = n - q$.
By (5.5), $\dim(K \cap N^{\perp}) = n - q$. q.e.d.

Remark. More generally, $\dim(K \cap N^{\perp}) = \dim(K) + \dim(N \cap K^{\perp}) - \dim(N)$ whenever $\dim(K) < \infty$ and $\dim(N) < \infty$. The proof is similar.

Proposition 5.2. *If* $\dim(K) < \infty$ *and* $N \cap K^{\perp} = \{\theta_X\}$, *then*

$$PN^{\perp} = K^{\perp} \tag{5.10}$$

where P *is the orthogonal projection onto* $K^{\perp}$.

Proof. It suffices to show that any element $k' \in K^{\perp}$ is the projection of an element $x \in N^{\perp}$, i.e. that there exists $k \in K$ such that $k + k' \in N^{\perp}$.

Let $\{w_1, \ldots, w_q\}$ be a basis for N. By (5.7), $\{Aw_1, \ldots, Aw_q\}$ is a basis for AN and by (5.5), $\{A^*Aw_1, \ldots, A^*Aw_q\}$ spans a subspace $H' \subset K$ of dimension q.

We take $k = \sum_{i=1}^{q} \lambda_i A^* A w_i$, the λ_i being chosen such that:

$$\left(\sum_{i=1}^{q} \lambda_i A^* A w_i, w_j\right)_X = -(k', w_j)_X, \quad j = 1, \ldots, q.$$

As we have $(A^*Aw_i, w_j)_X = (Aw_i, Aw_j)_E$, it suffices to take as λ_i the solution (which exists and is unique) of the linear system:

$$\sum_{i=1}^{q} \lambda_i (Aw_i, Aw_j)_E = -(k', w_j)_X, \quad j = 1, \ldots, q. \tag{5.11}$$

q.e.d.

VI. Characterization of the Interpolating Spline-function

Again consider the situation of § II. Thus,

$$T \in \mathscr{L}[X, Y]; \quad N = \mathscr{N}(T); \quad \dim(N) = q \quad \text{and} \quad \dim(K) = n. \tag{6.1}$$

General assumptions are:

$$N \cap K^{\perp} = \{\theta_X\} \quad \text{and } \mathscr{R}(T) \text{ closed}. \tag{6.2}$$

Without loss of generality,

$$\mathscr{R}(T) = Y. \tag{6.3}$$

Proposition 6.1. *Assume* (6.2) *and* (6.3), *then*

$$TK^{\perp} \quad \textit{is closed.} \tag{6.4}$$

Moreover,

$$TK^{\perp} = F^{\perp}, \tag{6.5}$$

where:

$$F = T^{*-1}(K \cap N^{\perp}), \tag{6.6}$$

$$\dim(F) = n - q. \tag{6.7}$$

Proof.

(6.8) $$TK^\perp = \mathcal{R}(T_{K^\perp}).$$

By (3.2), (3.3), (4.7) and proposition 5.2:

(6.9) $$\mathcal{R}(T_{K^\perp}{}^*) = P\mathcal{R}(T^*) = PN^\perp = K^\perp,$$

which is a closed subspace. By (3.3), $\mathcal{R}(T_{K^\perp})$ is closed. Thus, (6.4) is proved. By (3.2), T^{*-1} exists. Let $M = K^\perp$ in (3.6):

(6.10) $$(TK^\perp)^\perp = T^{*-1}(N^\perp \cap K) = F,$$

which yields (6.5), (6.6). Proposition 5.1 implies (6.7). q.e.d.

By (5.9):

(6.11) $$H = K \cap N^\perp = A^*(AN)^\perp.$$

This is useful for calculation. Construct a basis $\{b_1, \ldots, b_{n-q}\}$ for $B = (AN)^\perp \subset E$. Use (5.3) to define:

(6.12) $$h_i = A^* b_i = \sum_{j=1}^{n} b_i^j k_j, \quad i = 1, \ldots, n-q, \quad \text{where} \quad b_i = [b_i^1, \ldots, b_i^n] \in E.$$

By (5.5) and (6.11), $\{h_1, \ldots, h_{n-q}\}$ is a basis for H.

Let

(6.13) $$f_i = T^{*-1} h_i, \quad i = 1, \ldots, n-q.$$

Then $\{f_1, \ldots, f_{n-q}\}$ is a basis for F. By (2.4) and (6.5), $TK_r^\perp$ is a translate of $F^\perp$:

(6.14) $$F^\perp = \{y \in Y: (f_i, y)_Y = 0, \ i = 1, \ldots, n-q\}.$$

More precisely, by (2.1), (6.12) and (6.13):

(6.15) $$TK_r^\perp = F_r^\perp$$

with:

(6.16) $$F_r^\perp = \{y \in Y: (f_i, y)_Y = (b_i, r)_E, \quad i = 1, \ldots, n-q\}.$$

The following theorem expresses the complete solution of the minimization problem:

Theorem 6.2. *Assume* (6.2) *and* (6.3). *For each* $r \in E$, *there exists a unique* $\sigma \in X$ *satisfying* (2.2). *It is the unique element of* X *such that:*

(6.17) $$\sigma \in K_r^\perp,$$

(6.18) $$T\sigma = \sum_{j=1}^{n-q} \lambda_j f_j \in F.$$

The λ_j *satisfy the linear algebraic system:*

(6.19) $$\sum_{j=1}^{n-q} \lambda_j (f_i, f_j)_Y = (b_i, r)_E, \quad i = 1, \ldots, n-q.$$

Proof. By (6.9) we can apply proposition 2.1. By (2.6) and (6.5) we have (6.18). The linear system (6.19) is equivalent to $T\sigma \in TK_r^\perp$ (by (6.15), (6.16) and (6.18)). q.e.d.

VII. Examples for the Construction of Interpolating Spline-functions

For the effective construction, we can consider four steps:

Step 1. Determination of a basis for $H = K \cap N^\perp$. By proposition 5.1 it suffices to find $n-q$ linearly independent elements of K,

$$h_i = \sum_{j=1}^{n} b_i^j k_j, \quad i = 1, \ldots, n-q, \tag{7.1}$$

which are orthogonal to N, where $\{b_1, \ldots, b_{n-q}\}$ is a basis for $B = (A N)^\perp$.

Step 2. Determination of the $f_j = T^{*-1}(h_j)$ which span F.

Step 3. We then know that $f = T\sigma = \sum_{i=1}^{n-q} \lambda_i f_i$. We solve the linear system of $n-q$ equations of theorem 6.2. In practice this system is often well-conditioned (symmetrical matrix $(f_i, f_j)_Y$, often very sparse, with preponderant diagonal).

Step 4. We determine $\sigma \in K_r^\perp$ such that $T\sigma = f$. This latter step, which seems to be elementary may provide difficulties; whenever possible, one should proceed locally when satisfying the conditions imposed on σ (when the functionals k_i are of local type).

Example 1. Spline-functions by Point Evaluation

First, we go back to the example of § I.

In order to simplify, we set $q = 3$. Thus,

$$X = H^3[a, b], \qquad Y = H^0[a, b], \qquad T = D^3.$$

The functionals k_i are defined by:

$$(k_i, f)_3 = f(x_i), \quad i = 1, \ldots, n. \tag{7.2}$$

1. As functionals h_i, we can take the functionals δ_i^3, divided differences of order 3 with respect to the abscissae $x_i, x_{i+1}, x_{i+2}, x_{i+3}$, $(i = 1, \ldots, n-3)$:

$$h_i = \delta_i^3 = b_i^i \cdot k_i + b_i^{i+1} \cdot k_{i+1} + b_i^{i+2} \cdot k_{i+2} + b_i^{i+3} \cdot k_{i+3} \tag{7.3}$$

which effectively take the value zero on $\mathcal{N}(T) = \{\text{polynomials of degree } 2\}$.

2. We know that:

$$\delta_i^3 f = \int_a^b \Psi_i(t) \cdot f^{(3)}(t)\, dt \tag{7.4}$$

where Ψ_i is the kernel function of the divided difference. Thus:

$$\delta_i^3 f = (h_i, f)_3 = (\Psi_i, f^{(3)})_0 = (\Psi_i, Tf)_0. \tag{7.5}$$

Hence we have $h_i = T^* \Psi_i$.

So, $\{\Psi_1, \ldots, \Psi_{n-3}\}$ represents the needed basis for F. We know that:

$$\Psi_i(t) = \frac{1}{2!} \delta_i^3 [(x-t)_+^2]. \tag{7.6}$$

We have $\Psi_i(t) = 0$ for $t \notin [x_i, x_{i+3}]$, and $\Psi_i(t)$ is composed of pieces of polynomials of degree 2 which agree at the x_i, along with their first derivatives.

3. We have:

$$\sigma^{(3)} = \sum_{i=1}^{n-3} \lambda_i \Psi_i. \tag{7.7}$$

Thus, $\sigma \in H^3$ is composed of pieces of polynomials of degree 5 which agree at the x_i up to the fourth derivative (included).

The matrix $[(\Psi_i, \Psi_j)_0]$ has a preponderant diagonal and we have

$$(\Psi_i, \Psi_j)_0 = 0 \quad \text{for } |i-j| \geqq 3. \tag{7.8}$$

We solve:

$$\sum_{j=1}^{n-3} \lambda_j (\Psi_i, \Psi_j)_0 = c_i, \qquad i = 1, \ldots, n-3 \tag{7.9}$$

with:

$$c_i = \sum_{j=i}^{i+3} b_i^j r_j, \qquad i = 1, \ldots, n-3. \tag{7.10}$$

4. We have obtained:

$$\sigma^{(3)}(x_i) = \sum_{\substack{j=1 \\ |i-j|<3}}^{n-3} \lambda_j \Psi_j(x_i); \qquad \sigma^{(4)}(x_i) = \sum_{\substack{j=1 \\ |i-j|<3}}^{n-3} \lambda_j \cdot \Psi_j'(x_i). \tag{7.11}$$

The values $\sigma^{(1)}(x_i), \sigma^{(2)}(x_i)$, $i = 1, \ldots, n$, are then determined by integrating 3 times the function $\sigma^{(3)}$ and using 3 conditions $\sigma(x_j) = r_j$ in the neighbourhood of x_i (in the interval (x_i, x_{i+1}) the spline-function, which is a polynomial of degree 5, is exactly determined by the 6 values:

$$\sigma(x_i), \sigma^{(1)}(x_i), \sigma^{(2)}(x_i), \sigma(x_{i+1}), \sigma^{(1)}(x_{i+1}), \sigma^{(2)}(x_{i+1})). \tag{7.12}$$

Example 2. Spline-functions by Local Integrals

It happens frequently, especially with experimental measuring, that we do not know the value of a function at a given point, but can determine its mean value over an interval. Hence the usefulness of the spline-function which we are going to introduce:

$$X = H^2[a, b]; \qquad Y = H^0[a, b]; \qquad T = D^2.$$

Define the functionals k_i by:

$$(k_i, x)_2 = \frac{1}{t_{i+1} - t_i} \int_{t_i}^{t_{i+1}} x(t)\, dt, \qquad i = 1, \ldots, n, \tag{7.13}$$

with $a \leqq t_1 < t_2 < \cdots < t_{n+1} \leqq b$.

1. If $\xi(t)$ denotes an indefinite integral of $x(t)$, then we have in fact: $(k_i, x)_X = \delta_i^1 \xi$, a divided difference of order 1 of ξ with respect to the abscissae t_i, t_{i+1}.

We consider the functional h_i defined by:

$$(h_i, x)_2 = \delta_i^3 \xi, \tag{7.14}$$

where $\delta_i^3 \xi$ is the divided difference of order 3 of ξ with respect to $t_i, t_{i+1}, t_{i+2}, t_{i+3}$. We can express δ_i^3 in terms of $k_i = \delta_i^1$, $k_{i+1} = \delta_{i+1}^1$ and $k_{i+2} = \delta_{i+2}^1$:

$$h_i = \frac{1}{t_{i+3} - t_i} \left[\frac{1}{t_{i+2} - t_i} k_i - \left(\frac{1}{t_{i+3} - t_{i+1}} + \frac{1}{t_{i+2} - t_i} \right) k_{i+1} + \frac{1}{t_{i+3} - t_{i+1}} k_{i+2} \right] \tag{7.15}$$

$$i = 1, \ldots, n-2.$$

We have then:

(7.16) $(h_i, x)_2 = 0$ when $x \in \mathcal{N}(D^2) = \{\text{polynomials of degree } 1\}$.

Hence $\{h_1, \ldots, h_{n-2}\}$ is a basis of H.

2. By (7.4) we have:

$$\delta_i^3 \xi = (h_i, x)_2 = \int_a^b \Psi_i(t) \cdot \xi^{(3)}(t)\, dt = \int_a^b \Psi_i(t) \cdot x''(t)\, dt, \tag{7.17}$$

$$(h_i, x)_2 = (\Psi_i, x'')_0 = (\Psi_i, Tx)_0. \tag{7.18}$$

Hence:

$$h_i = T^* \Psi_i, \qquad i = 1, \ldots, n-2, \tag{7.19}$$

with Ψ_i defined by (7.6).

3. We have:

$$\sigma'' = \sum_{i=1}^{n-2} \lambda_i \Psi_i. \tag{7.20}$$

We see that $\sigma(t)$ is composed of pieces of polynomials of degree 4 which agree at the t_i up to the third derivative (included).

We have $(\Psi_i, \Psi_j)_0 = 0$ when $|i-j| \geqq 3$.

We solve:

$$\sum_{j=1}^{n-2} \lambda_j (\Psi_i, \Psi_j) = d_i, \qquad i = 1, \ldots, n-2, \tag{7.21}$$

with

$$d_i = \frac{1}{t_{i+3}-t_i} \left[\frac{1}{t_{i+2}-t_i} r_i - \left(\frac{1}{t_{i+3}-t_{i+1}} + \frac{1}{t_{i+2}-t_i} \right) r_{i+1} + \frac{1}{t_{i+3}-t_{i+1}} r_{i+2} \right]. \tag{7.22}$$

4. In each interval $[t_i, t_{i+1}]$ we know:

$$\sigma^{(2)}(t_i),\ \sigma^{(2)}(t_{i+1}),\ \sigma^{(3)}(t_i),\ \sigma^{(3)}(t_{i+1}) \quad \text{and} \quad \int_{t_i}^{t_{i+1}} \sigma(t)\, dt.$$

The values $\sigma(t_i)$, $\sigma'(t_i)$, $i = 1, \ldots, n+1$, are then determined by integrating 2 times the function $\sigma^{(2)}$ and using 2 conditions $(k_j | \sigma) = r_j$ in the neighbourhood of t_i. (In the interval (t_i, t_{i+1}) the spline-function, which is a polynomial of degree 4, is exactly determined by the 5 values:

$$\left(\int_{t_i}^{t_{i+1}} \sigma(t)\, dt,\ \sigma(t_i),\ \sigma(t_{i+1}),\ \sigma'(t_i),\ \sigma'(t_{i+1}) \right). \tag{7.23}$$

Example 3. Fourier Spline-functions

$$X = H^2[-1, +1], \qquad Y = H^0[-1, +1], \qquad T = D^2.$$

Let $P_0, P_1, \ldots, P_{n-1}$ be the first n polynomials of Legendre, orthonormal on $[-1, +1]$:

$$\int_{-1}^{+1} P_i(t) \cdot P_j(t)\, dt = \delta_{ij}. \tag{7.24}$$

We define the functionals k_i by:

$$(k_i, x)_2 = \int_{-1}^{+1} P_{i-1}(t) \cdot x(t)\, dt, \qquad i = 1, \ldots, n. \tag{7.25}$$

1. We can take

$$h_i = k_{i+2}, \quad i = 1, \ldots, n-2.$$

By (7.24) we have

(7.26) $$(h_i, x)_2 = 0 \quad \text{when} \quad x \in \mathcal{N}(D^2).$$

2. We have:

(7.27) $$(h_i, x)_2 = \int_{-1}^{+1} P_{i+1}(t) \cdot x(t)\, dt = \int_{-1}^{+1} Q_{i+1}(t) \cdot x''(t)\, dt = (Q_{i+1}, Tx)_0,$$

$$i = 1, \ldots, n-2,$$

with:

$$Q_{i+1}(t) = \int_t^1 (u-t)\, P_{i+1}(u)\, du.$$

The $f_i \in Y$ are thus represented by the Q_{i+1} ($i = 1, \ldots, n-2$) which are polynomials of degree $i+3$ satisfying:

$$Q_{i+1}(\pm 1) = Q'_{i+1}(\pm 1) = 0.$$

3. We have:

(7.28) $$f = \sigma''(t) = \sum_{i=1}^{n-2} \lambda_i Q_{i+1}(t).$$

Thus, the solution is a polynomial of degree $n+3$ which can be written in the form

(7.29) $$\sigma(t) = \sum_{i=0}^{n-1} r_{i+1} P_i(t) + \sum_{i=n}^{n+3} \gamma_i P_i(t)$$

(the r_j are the given numbers: $(k_j, \sigma)_X = r_j$, $j = 1, \ldots, n$).

The solution σ satisfies $\sigma''(\pm 1) = \sigma'''(\pm 1) = 0$.

In order to determine the λ_i, we solve the linear system of dimension $n-2$:

(7.30) $$\sum_{j=1}^{n-2} \lambda_j (Q_{j+1}, Q_{i+1}) = r_{i+2}, \quad i = 1, \ldots, n-2.$$

Note that $(Q_{j+1}, Q_{i+1}) = 0$ for $|i-j| > 4$.

If $R_{i+1}(t)$ designates the second primitive of $Q_{i+1}(t)$ which is orthogonal to P_0 and P_1, then:

(7.31) $$\sigma(t) = r_1 P_0(t) + r_2 P_1(t) + \sum_{i=1}^{n-2} \lambda_i R_{i+1}(t).$$

VIII. General Smoothing Spline-functions

Let us go back first to the introductory example of § I: If the given values r_i comprise errors (experimental or otherwise) it is not necessary to satisfy exactly the relations $f(x_i) = r_i$, $i = 1, \ldots, n$.

On the contrary, it is more interesting to make a compromise between the approximation of the data characterized by:

(8.1) $$E(f) = \sum_{i=1}^{n} \left(f(x_i) - r_i\right)^2$$

and the smoothness of the solution characterized by:

(8.2) $$S(f) = \int_a^b \left(f^{(q)}(t)\right)^2 dt.$$

Let

(8.3) $$M(f) = S(f) + \varrho E(f) \quad \text{with} \quad \varrho > 0.$$

We know that the element $s \in H^q$ (which we shall call *smoothing spline-function*) such that:

(8.4) $$M(s) = \min_{f \in H^q} M(f)$$

exists and is unique (for $n \geq q$). Once again, it is composed of pieces of polynomials of degree $2q-1$ which agree at the x_i up to the $(2q-2)^{\text{nd}}$ derivative (included). It also satisfies (1.5) and can be written according to (1.6).

We shall study now the problem of the characterization and the construction of the spline-function s within the more general framework already used in § II: Using the same notations as in § II. we shall call again *smoothing spline function* (relative to T, $\{k_1, \ldots, k_n\}$, $\{r_1, \ldots, r_n\}$ and $\varrho > 0$) any element $s \in X$ which satisfies (generalizing (8.4)):

(8.5) $$M(s) = \min_{x \in X} M(x)$$

with:

(8.6) $$M(x) = \|Tx\|_Y^2 + \varrho \sum_{i=1}^{n} \left((k_i, x)_X - r_i\right)^2.$$

Let $Z = X \times E$ the Hilbert space with inner product:

(8.7) $$(z_1, z_2)_Z = (y_1, y_2)_Y + \varrho (e_1, e_2)_E \quad \text{with} \quad z_1 = [y_1, e_1], \quad z_2 = [y_2, e_2].$$

Let L be the continuous linear operator on X into Z defined by:

(8.8) $$Lx = [Tx, Ax] \in Z,$$

where A is defined by (5.1).

Define $a \in Z$ by

(8.9) $$a = [\theta_Y, r],$$

where θ_Y is the origin of Y. Then

(8.10) $$M(x) = \|Lx - a\|_Z^2.$$

So, we want to determine $s \in X$ such that:

(8.11) $$\|Ls - a\|_Z = \operatorname*{Min}_{x \in X} \|Lx - a\|_Z.$$

Proposition 8.1. *If LX is closed and $\mathcal{N}(T) \cap K^\perp = \{\theta_X\}$ then, for each $r \in E$, there exists a unique spline function $s \in X$ satisfying* (8.11) *which is determined by the condition*

(8.12) $$Ls - a \in (LX)^\perp.$$

Proof. We want to determine $p = Ls$ of LX at minimum distance of $a \in Z$. The subspace LX being closed, the solution p exists and is unique: it is the projection of $a \in Z$ upon LX; thus p is entirely characterised by

(8.13) $$p - a \in (LX)^\perp, \qquad p \in LX.$$

By the hypothesis:

(8.14) $$\mathcal{N}(T) \cap K^\perp = \mathcal{N}(T) \cap \mathcal{N}(A) = \{\theta_X\},$$

L is a one-to-one operator. So, there exists a unique $s \in X$ such that $Ls = p$. q.e.d.

It will be shown that LX is closed whenever $\mathcal{N}(T) \cap K^\perp = \{\theta_X\}$ and $\mathcal{R}(T)$ is closed. The determination of $p = Ls$ will be reduced to the solution of a finite algebraic system.

Proposition 8.2. *Assume* (6.2) *and* (6.3); *then*

(8.15) $$LX = G^\perp$$

where

(8.16) $$G = \mathcal{N}(L^*),$$

(8.17) $$\dim(G) = n - q.$$

Proof. Let $z = [z_Y, z_E]$ an element of Z.

By (3.1) we have

(8.18) $$L^* z = T^* z_Y + \varrho A^* z_E.$$

Thus by (3.2) and (3.3):

(8.19) $$L^* Z = \mathcal{R}(T^*) + \mathcal{R}(A^*) = N^\perp + K.$$

From proposition 5.2, it follows immediately that:

(8.20) $$N^\perp + K = X.$$

As $\mathcal{R}(L^*) = X$, according to the closed range theorem (3.3)

(8.21) $$LX \quad \text{is closed},$$

and by (3.2),

(8.22) $$LX = \mathcal{R}(L) = \mathcal{N}(L^*)^\perp.$$

It remains to be shown that $G = \mathcal{N}(L^*)$ is of dimension $n - q$: In fact, we have $L^* z = 0$ iff $x = T^* z_Y = -\varrho \cdot A^* z_E$, which is possible only for an element x such that

(8.23) $$x \in T^* Y \cap \varrho A^* E = N^\perp \cap K = H$$

which is of dimension $n - q$ (proposition 5.1). As T^* and A^* are one-to-one, the kernel G of L^* is of dimension $n - q$ and we can take the following basis:

(8.24) $$g_i = \left[f_i, \frac{-b_i}{\varrho}\right], \qquad i = 1, \ldots, n - q$$

with $f_i = T^{*-1} h_i$ and $b_i = A^{*-1} h_i$ (by (6.12) and (6.13)). q.e.d.

Theorem 8.3. *Assume* (6.2) *and* (6.3). *For each* $r \in E$ *there exists a unique solution* $s \in X$ *satisfying* (8.11) *which is the unique element of* X *such that:*

(8.25) $$Ls - a = \sum_{j=1}^{n-q} \mu_j g_j \in G.$$

The μ_j *satisfy the linear algebraic system:*

(8.26) $$\sum_{j=1}^{n-q} \mu_j (g_j, g_i)_Z = -(a, g_i)_Z, \qquad i = 1, \ldots, n - q.$$

Proof. By proposition (8.2), $\mathscr{R}(L)$ is closed and we can apply proposition (8.1). The condition (8.25) follows from (8.12) and (8.15). The linear system (8.26) is equivalent to

$$p = Ls = \sum_{j=1}^{n-q} \mu_j g_j + a \in G^{\perp}. \tag{8.27}$$ q.e.d.

IX. Examples for the Construction of Smoothing Spline-functions

The steps 1 and 2 of § VII remain unchanged.

Step 3'. We know that $g = p - a = \sum_{i=1}^{n-q} \mu_i g_i$ where the μ_i satisfy the linear system (8.26).

We recall that

$$(g_j, g_i)_Z = (f_j, f_i)_Y + \frac{1}{\varrho}(b_j, b_i)_E \tag{9.1}$$

and by (8.9) and (8.24):

$$-(a, g_i)_Z = (r, b_i)_E. \tag{9.2}$$

The matrix $(g_j, g_i)_Z$ is often very similar in form to the matrix $(f_j, f_i)_Y$ and is usually well-conditioned.

Step 4'. The equation $p = Ls = a + \sum_{i=1}^{n-q} \mu_i g_i$ yields both

$$Ts = \sum_{i=1}^{n-q} \mu_i f_i \tag{9.3}$$

and

$$As = r - \frac{1}{\varrho} \sum_{i=1}^{n-q} \mu_i b_i. \tag{9.4}$$

Thus, we are exactly at the same point as at step 4 of § VII for obtaining s. Note that s is always of the same form as σ (simply corresponding to different values of r_i).

We return to the examples presented in § VII, using the same notations. We shall indicate briefly the modifications for step 3'.

Example 1. Spline-functions by Point Evaluation

We obtain the μ_j by solving the linear system:

$$\sum_{j=1}^{n-3} \beta_{kj} \mu_j = c_k, \qquad k = 1, \ldots, n-3 \tag{9.5}$$

with

$$\beta_{kj} = (\Psi_k, \Psi_j)_0 + \frac{1}{\varrho} \sum_{i=1}^{n} b_k^i b_j^i, \tag{9.6}$$

where

$$b_j^i = \begin{cases} \dfrac{1}{\prod\limits_{\substack{k=j \\ k \neq i}}^{j+3} (x_k - x_i)} & \text{if } j \leq i \leq j+3, \\ 0 & \text{otherwise}. \end{cases} \tag{9.7}$$

(These are the coefficients of the divided difference (7.3).)

Note that the matrix β_{kj} satisfies:

(9.8) $$\beta_{kj} = 0 \quad \text{when} \quad |k-j| \geqq 4.$$

We have:

(9.9) $$s'''(t) = \sum_{j=1}^{n-3} \mu_j \Psi_j(t)$$

and

(9.10) $$(k_i, s)_X = s(x_i) = r_i - \frac{1}{\varrho} \sum_{j=1}^{n-3} \mu_j b_j^i, \qquad i = 1, \ldots, n.$$

Example 2. Spline-functions by Local Integrals

We obtain the μ_j by solving the linear system:

(9.11) $$\sum_{j=1}^{n-2} \beta_{kj} \mu_j = d_k, \qquad k = 1, \ldots, n-2,$$

where the β_{kj} are computed by (9.6) with (see (7.22)):

(9.12) $$b_j^i = \begin{cases} \dfrac{1}{(t_{j+3}-t_j)(t_{j+2}-t_j)} & \text{if} \quad i = j \\ \dfrac{-1}{t_{j+3}-t_j} \left(\dfrac{1}{t_{j+3}-t_{j+1}} + \dfrac{1}{t_{j+2}-t_j} \right) & \text{if} \quad i = j+1 \\ \dfrac{1}{(t_{j+3}-t_j)(t_{j+3}-t_{j+1})} & \text{if} \quad i = j+2 \\ 0 & \text{otherwise}. \end{cases}$$

Note that the matrix β_{kj} has the same general form as the matrix $(\Psi_k, \Psi_j)_0$:

(9.13) $$\beta_{kj} = 0 \quad \text{when} \quad |k-j| \geqq 3.$$

We have

(9.14) $$s''(t) = \sum_{j=1}^{n-2} \mu_j \Psi_j(t)$$

and

(9.15) $$(k_i, s)_X = \frac{1}{t_{i+1}-t_i} \int_{t_i}^{t_{i+1}} s(t)\, dt = r_i - \frac{1}{\varrho} \sum_{j=1}^{n-2} \mu_j b_j^i, \qquad i = 1, \ldots, n.$$

Example 3. Fourier Spline-functions

We obtain the μ_j by solving the linear system:

(9.16) $$\sum_{j=1}^{n-2} \beta_{kj} \mu_j = r_{k+2}, \qquad k = 1, \ldots, n-2,$$

with:

(9.17) $$\beta_{kj} = (Q_{k+1}, Q_{j+1}) \quad \text{for} \quad k \neq j \quad \text{and} \quad \beta_{kk} = (Q_{k+1}, Q_{k+1}) - \frac{1}{\varrho}.$$

We have:

(9.18) $$s''(t) = \sum_{i=1}^{n-2} \mu_i \cdot Q_{i+1}(t),$$

and

$$(9.19)\quad \begin{cases} (k_i, s)_X = \int_{-1}^{+1} P_{i-1}(t)\, s(t)\, dt = r_i, & \text{for } i = 1, 2, \\ (k_i, s)_X = \int_{-1}^{+1} P_{i-1}(t)\, s(t)\, dt = r_i - \frac{1}{\varrho} \cdot \mu_{i-2} \cdot r_i, & \text{for } i = 3, 4, \ldots, n. \end{cases}$$

The solution $s(t)$ can be written:

$$(9.20)\qquad s(t) = r_1 P_0(t) + r_2 P_1(t) + \sum_{i=2}^{n-1} s_{i+1} P_i(t) + \sum_{i=n}^{n+3} \gamma_i' P_i(t)$$

with $s''(\pm 1) = s'''(\pm 1) = 0$, or else in the form:

$$(9.21)\qquad s(t) = r_1 P_0(t) + r_2 P_1(t) + \sum_{i=1}^{n-2} \mu_i R_{i+1}(t).$$

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