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SMOOTHING SPLINE IN A CONVEX CLOSED SET OF HILBERT SPACE

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A characterisation of a smoothing spline is sought in a convex closed set C of Hilbert space: $\min\{\alpha\|Tx\|_Y^2 + \|Ax - z\|_Z^2, x \in C\}$, T and A are linear operators. A representation of the solution is obtained in the terms of the kernels of the above operators, of the dual operators T^*, A^* and of the dual cone C^0. A particular case is considered when T is the differential operator and A is the operator-trace of a function.

Let X, Y, Z be Hilbert spaces with scalar products respectively $(,)_X, (,)_Y, (,)_Z$. We are given linear bounded operators

$$A : X \to Z, \quad T : X \to Y.$$

Consider the operator equation $Ax = z_0, z_0 \in Z$.

1. If $A^{-1}(z_0) \neq \emptyset$, then $\sigma \in X$ is called *an interpolating spline*, if the following minimum is reached

$$(1) \qquad \|T\sigma\|_Y^2 = \min_{x \in A^{-1}(z_0)} \|Tx\|_Y^2.$$

2. If $A^{-1}(z_0) = \emptyset$, we introduce a real parameter $\alpha > 0$ and construct a quadratic functional

$$(2) \qquad \phi_\alpha(x) = \alpha\|Tx\|_Y^2 + \|Ax - z_0\|_Z^2.$$

We say that $\sigma_* \in X$ is *a smoothing spline*, if

$$(3) \qquad \phi_\alpha(\sigma_*) = \min_{x \in X} \phi_\alpha(x).$$

Characterisations of the solutions of problems (1) and (3) are given in [5].

A certain shape of the interpolating or smoothing spline is required in many applied problems. The characterisation of such conditions can be often described by a set $C \subset X$, which is convex and closed.

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Chui, Deutsch and Ward give a characterisation of the solution of the problem for an interpolating spline in a convex set of Hilbert space ([**3**, **4**])

$$\min_{Ax=z_0,\ x\in C} \|x\|^2. \tag{4}$$

In [**2**] a particular case of monotonicity is considered for both interpolating and smoothing splines. The characterisation is done from the point of view of a general optimisation problem in the terms of the Frechet-derivative and the polar cone.

We shall consider here the problem of finding a smoothing spline in a convex closed set of Hilbert space. That is, σ_* is sought so that

$$\phi_\alpha(\sigma_*) = \min_{x\in C\subset X} \phi_\alpha(x), \tag{5}$$

where $\phi_\alpha(x)$ is the functional in (2). This problem arises for example, if the data are corrupted by noise and one does not require exact interpolation, but a special form of spline is required.

A new linear operator L can be defined ([**5**]), which is acting on $F = Y \times Z$. If $f_1 = [y_1, z_1]$, $y_1 \in Y$, $z_1 \in Z$, $f_2 = [y_2, z_2]$, $y_2 \in Y$, $z_2 \in Z$, we define a scalar product in F by

$$(f_1, f_2)_F = \big([y_1, z_1], [y_2, z_2]\big)_F := \alpha(y_1, y_2)_Y + (z_1, z_2)_Z.$$

Let L be the linear bounded operator

$$L : X \to F, Lx = [Tx, Ax],$$

and let $a = [0_Y, z_0]$ be an element of F.

Lemma 1. *$\phi_\alpha(x) = \|Lx - a\|_F^2$, where $a = [0_Y, z_0]$.*

Proof: By the definitions

$$\begin{aligned}(Lx - a, Lx - a)_F &= \big([Tx, Ax] - [0_Y, z_0], [Tx, Ax] - [0_Y, z_0]\big)_F \\ &= \big([Tx, Ax - z_0], [Tx, Ax - z_0]\big)_F = \alpha(Tx, Tx)_Y + (Ax - z_0, Ax - z_0)_Z \\ &= \alpha\|Tx\|^2 + \|Ax - z_0\|^2 = \phi_\alpha(x).\end{aligned}$$

Therefore $\phi_\alpha(x) = (Lx - a, Lx - a)_F = \|Lx - a\|_F^2$. ∎

Then the problem (5) is equivalent to

$$\min_{f\in K} \|f - a\|^2, \tag{6}$$

where $K = L(C) = \big\{[y, z] \in Y \times Z : y = Tx, z = Ax, x \in C\big\}$.

Denote the kernels of T and A respectively by

$$\ker T = \{x \in X : Tx = 0_Y\}, \ \ker A = \{x \in X : Ax = 0_Z\}.$$

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Lemma 2. *If T and A are linear bounded operators and $\ker T \cap \ker A = \{0_X\}$, then L is a linear bounded continuous operator and $\ker L = \{0_X.\}$*

Proof: L is a linear bounded operator, obviously. It follows it is continuous.

Let us show that $\ker L = \{0_X\}$. If $x \in \ker L$, that is, $Lx = 0_F$, then $Lx = [Tx, Ax] = [0_Y, 0_Z]$, therefore $Tx = 0_Y, Ax = 0_Z$, and $x \in \ker T \cap \ker A = 0_X$; or $\ker L = 0_X$.

The following lemma follows from the inverse operator theorem.

Lemma 3. *If T and A are linear bounded operators, $\ker T \cap \ker A = 0_X$, and $L(X)$ is closed, then there exists $L^{-1} : L(X) \subset F \to X$ and L^{-1} is a linear bounded continuous operator, too.*

Here $L(X) = \{[y, z] : y = Tx, z = Ax, x \in X\}$.

We shall find conditions for closeness of $L(X)$ to be closed.

Lemma 4. *$L(X)$ is closed if and only if $\ker T + \ker A$ is closed.*

Proof: $L(X)$ is closed if and only if $L^*(F) = T^*(Y) + A^*(Z)$ is closed in X, if and only if $\ker T^{\perp} + \ker A^{\perp}$ is closed if and only if $\ker T + \ker A$ is closed. ∎

Lemma 5. *If C is a closed convex subset of X, $\ker T \cap \ker A = \{0_X\}$, and $\ker T + \ker A$ is closed, then $K = L(C)$ is a closed and convex subset of F.*

Proof: Let $f_1, f_2 \in L(C), \lambda_1 \geqslant 0, \lambda_2 \geqslant 0, \lambda_1 + \lambda_2 = 1$. We shall show that $\lambda_1 f_1 + \lambda_2 f_2 \in L(C)$,too. There exists unique $x_1 \in C : f_1 = Lx_1$, and $x_2 \in C : f_2 = Lx_2$. We have $\lambda_1 f_1 + \lambda_2 f_2 = \lambda_1 Lx_1 + \lambda_2 Lx_2 = L(\lambda_1 x_1 + \lambda_2 x_2) \in L(C)$, because $\lambda_1 x_1 + \lambda_2 x_2 \in C$.

Let's show, that $L(C)$ is closed. If $\{f_n\} \to f, f_n \in L(C)$, we shall show that $f \in L(C)$.

There exists unique $x_n \in C : f_n = Lx_n, Lx_n \to f$. Applying the inverse continuous operator L^{-1}, it follows $L^{-1}Lx_n \to L^{-1}f = x$.

So we have $x_n \to x$, but C is closed, therefore $x \in C$. It means $f = Lx \in L(C)$. ∎

Theorem 1. *If C is a convex closed subset of X, $\ker T \cap \ker A = 0_X$ and $\ker T + \ker A$ is closed, then the problem* (5) *has the unique solution*

$$\sigma_* = L^{-1} P_{L(C)}(a),$$

where $P_{L(C)}(a)$ denotes the orthogonal projection of a on $L(C)$.

Proof: A classical result ([**5**, Theorem 2.1.2]) shows, that there exist unique solution of the problem (6) $f_* \in K$, such that

$$\|f_* - a\|^2 = \min_{f \in K} \|f - a\|^2.$$

The point $f_* \in L(C)$, in which $\min \|f - a\|$ is reached, is the orthogonal projection of a on $L(C)$, that is, $f_* = P_{L(C)}(a)$. But $f_* = L\sigma_*$ for some σ_*, and L is converse, (in according with Lemma 3 and 4), therefore the solution has the form

$$\sigma_* = L^{-1}\big(P_{L(C)}(a)\big). \tag{7}$$

∎

Further we shall omit the brackets in $L(C)$ and denote $LC := L(C)$. Define the dual operator A^* of A by

$$(z, Ax) = (A^* z, x)$$

for all $z \in Z, x \in X$.

We denote the dual cone of C by

$$C^0 = \{x \in X : (x, y) \leqslant 0, \forall y \in C\}.$$

It is easy to see, that

$$f_* = P_{LC}(a) \text{ if and only if } a - f_* \in (LC - f_*)^0 = (LC)^0 \cap f_*^{\perp}. \tag{8}$$

Theorem 2. *Problem* (5) *has the unique solution* σ_* *if and only if*

$$-\alpha T^* T \sigma_* + A^*(z_0 - A\sigma_*) \in C^0, \tag{9}$$

and

$$\Phi_\alpha(\sigma_*) = (z_0 - A\sigma_*, z_0). \tag{10}$$

Proof: By (8), $a - f_* \in (LC)^0$ means, that

$$(a - f_*, L\sigma) \leqslant 0, \forall \sigma \in C.$$

But $f_* \in L(C)$, therefore there exist unique σ_* such that $f_* = L\sigma_* = [T\sigma_*, A\sigma_*]$. Then

$$\begin{aligned}(a - f_*, L\sigma) &= \big([0_Y, z_0] - [T\sigma_*, A\sigma_*], [T\sigma, A\sigma]\big) = \big([-T\sigma_*, z_0 - A\sigma_*], [T\sigma, A\sigma]\big) \\ &= -\alpha(T\sigma_*, T\sigma) + (z_0 - A\sigma_*, A\sigma) \leqslant 0.\end{aligned} \tag{11}$$

Therefore

$$(-\alpha T^* T\sigma_*, \sigma) + \big(A^*(z_0 - A\sigma_*), \sigma\big) \leqslant 0, \ \sigma \in C.$$

This means, that

$$-\alpha T^* T\sigma_* + A^*(z_0 - A\sigma_*) \in C^0,$$

and (9) has been proved.

Again from (8) $a - f_* \in f_*^{\perp}$. It follows, that $(a - f_*, f_*)_F = 0$. But $f_* = (T\sigma_*, A\sigma_*)$, so

$$\begin{aligned}\big([0_Y, z_0] - [T\sigma_*, A\sigma_*], [T\sigma_*, A\sigma_*]\big) &= \big([-T\sigma_*, z_0 - A\sigma_*], [T\sigma_*, A\sigma_*]\big) \\ &= -\alpha\|T\sigma_*\|^2 + (z_0 - A\sigma_*, A\sigma_*) \\ &= -\alpha\|T\sigma_*\|^2 - (A\sigma_* - z_0, A\sigma_* - z_0) - (A\sigma_* - z_0, z_0) \\ &= -\Phi_\alpha(\sigma_*) - (A\sigma_* - z_0, z_0) = 0.\end{aligned}$$

Therefore $\Phi_\alpha(\sigma_*) = (z_0 - A\sigma_*, z_0)$. Note that equality in (11) is reached only for the solution σ_*. We obtain then equation (10), and the theorem has been proved. □

We shall look for the solution of problem (5) in a proper basis.

Let $k_1, k_2, \ldots, k_N$ be linearly independent elements of X, and $A : X \to Z = Z^N$. The action of the operator A may be represented by

$$A\sigma = \big((k_1, \sigma), (k_2, \sigma), \ldots, (k_N, \sigma)\big).$$

Let K be the space of linear combinations of $k_1, k_2, \ldots, k_N$. The dual operator satisfies

$$A^*\lambda = \sum \lambda_i k_i.$$

The Hilbert space Y may be represented as a direct sum

$$Y = (T \ker A) \oplus (T \ker A)^\perp.$$

For the solution $\sigma_* \in X$ there exists $y_0 \in T \ker A$, with $y_0 = Tx_0$ for some element $x_0 \in \ker A$, and there exists $y \in (T \ker A)^\perp$, so that

(12) $$T\sigma_* = y_0 + y = Tx_0 + y.$$

The following equations can be proved easily.

Lemma 6.

(1) $\ker A = K^\perp$.

(2) $(TK^\perp)^\perp = T^{*-1}(H)$, *where* $H = K \cap (\ker T)^\perp$.

(3) *If* $\ker T \cap \ker A = 0_X$ *and* $\dim \ker T = q < \infty$, *then*

$$\dim H = \dim K - \dim(\ker T) = N - q.$$

(4) $(T^{*-1}h)(t) = \big(h(x), G_+(x-t)\big)_X$, *where* $h \in (\ker T)^\perp$.

Here $G_+(x-t)$ *is the Green's function with* $TG_+(x-t) = \delta_t$, *and* $\delta_t(v) = v(t), v \in X$.

An algorithm for finding a basis in $(T \ker A)^\perp$ follows if we use Lemma 6.

(1) A basis for $H = K \cap (\ker T)^\perp$ is looked for

$$h_i = \sum_{j=1}^{N} h_{ij} k_j, i = 1, 2, \ldots, N - q.$$

(2) If $e_1, e_2, \ldots, e_q$ is a basis for $\ker T$, then

$$0 = (h_i, e_k) = \sum_{j=1}^{N} h_{ij}(k_j, e_k), i = 1, 2, \ldots, N - q, k = 1, 2, \ldots, q.$$

(3) $f_i = T^{*-1}(h_i), i = 1, 2, \ldots, N-q$ is a basis for $T^{*-1}(H) = (TK^\perp)^\perp = (T \ker A)^\perp$.

(4) For every $y \in (T \ker A)^\perp$ there exist $\lambda_1, \lambda_2, \ldots, \lambda_{N-q}$, so that

$$y = \sum_{i=1}^{N-q} \lambda_i f_i.$$

Now from (12) we have the representation

$$T\sigma_* = Tx_0 + \sum \lambda_i f_i. \tag{13}$$

Let's introduce the matrices

$$H = (h_{ij})_{i=1,\ldots,N-q}^{j=1,\ldots,N}, \quad F = \big((f_i, f_j)\big)_{i=1,\ldots,N-q}^{j=1,\ldots,N-q}. \tag{14}$$

$$\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_{N-q}), \quad r = (r_1, r_2, \ldots, r_N). \tag{15}$$

Lemma 7. *For every $y \in (T \ker A)^\perp$ there exists $r \in Z^N$, so that*

$$T^* y = A^* r, \quad r = \lambda H.$$

Proof: From the above there exist $\lambda_1, \lambda_2, \ldots, \lambda_{N-q}$, so that $y = \sum \lambda_i f_i$. Thus

$$T^*y = T^*\Big(\sum \lambda_i f_i\Big) = \sum \lambda_i (T^* f_i) = \sum \lambda_i h_i = \sum \lambda_i \sum h_{ij} k_j$$
$$= \sum \sum \lambda_i h_{ij} k_j = \sum r_j k_j = A^* r, r = (r_1, r_2, \ldots, r_N).$$

Here

$$r_j = \sum_{i=1}^{N-q} \lambda_i h_{ij},$$

or, using a matrix form,

$$r = \lambda H. \tag{16}$$

∎

Let us denote $v = A\sigma_* = \big((k_1, \sigma_*), \ldots, (k_N, \sigma_*)\big)$. There exists a relation between λ and v.

Lemma 8. $\lambda F = v H^T$.

Proof: We have in (13) $T\sigma_* = Tx_0 + \sum \lambda_i f_i$. Thus

$$(T\sigma_*, f_j) = (Tx_0, f_j) + \Big(\sum \lambda_i f_i, f_j\Big) = (x_0, T^* f_j) + \sum \lambda_i (f_i, f_j). \tag{17}$$

But $(x_0, T^* f_j) = (x_0, h_j) = 0$ because of $x_0 \in \ker A = K^\perp, h_j \in H \subset K$. On the other hand,

$$(T\sigma_*, f_j) = (\sigma_*, h_j) = \Big(\sigma_*, \sum h_{jl} k_l\Big) = \sum h_{jl} (k_l, \sigma_*) = \sum h_{jl} v_l. \tag{18}$$

Comparing the right sides of (17) and (18), it follows

$$\lambda F = vH^T. \tag{19}$$

□

Lemma 9. *If $e_1, e_2, \ldots, e_q$ is a basis for $\ker T$ and $B = (b_{j,k})_{j=1,2,\ldots,N}^{k=1,2,\ldots,q}$, with $b_{j,k} = (k_j, e_k)$, then $rB = 0$.*

Proof: From (2) and (1) of the algorithm above, it follows that

$$0 = \sum \lambda_i (h_i, e_k) = \sum \lambda_i \Big(\sum h_{ij} k_j, e_k \Big) = \sum \lambda_i h_{ij} (k_j, e_k) = \sum r_j b_{kj}, k = 1, 2, \ldots, q.$$

Therefore $rB = 0$. □

From the representation (13) of the solution and Lemma 7 it follows that there exist $x_0 \in \ker A$ and $r \in Z^N$, so that

$$T^* T \sigma_* = T^* T x_0 + A^* r.$$

The conditions (9) and (10) take the form

$$-\alpha T^* T x_0 + A^*(-\alpha r + z_0 - v) \in C^0,$$
$$\alpha \Big\| T x_0 + \sum \lambda_i f_i \Big\|^2 = (z_0 - v, v).$$

Let us remark

$$\Big\| T x_0 + \sum \lambda_i f_i \Big\|^2 = \|T x_0\|^2 + \sum \sum \lambda_i (f_i, f_j) \lambda_j = \|T x_0\|^2 + \lambda F \lambda^T.$$

The following theorem is a consequence of Lemmas 7, 8 and 9.

Theorem 3. *The solution σ_* of the problem* (5) *may be represented in the form*

$$T \sigma_* = T x_0 + \sum \lambda_i f_i, \quad x_0 \in \ker A,$$

if and only if x_0 and λ satisfy

$$-\alpha T^* T x_0 + A^*(-\alpha r + z_0 - v) \in C^0$$
$$\alpha \big(\|T x_0\|^2 + \lambda F \lambda^T \big) = (z_0 - v, v),$$

where $r \in Z^N, v \in Z^N$ are related to λ by

$$r = \lambda H, \quad \lambda F = v H^T, \quad rB = 0.$$

Let us consider problem (5) in the following situation. The knots

$$a = t_1 < t_2 < \ldots < t_N = b$$

and values $z_1, z_2, \ldots, z_N$ are given in the interval $[a,b]$. Let $X = W_2^n[a,b]$ be the Sobolev space of functions with the usual norm

$$\|f\|^2_{W_2^n} = \sum_{j=0}^{n} \|f^{(j)}\|^2_{L^2[a,b]}$$

Let $Y = L_2[a,b]$ be the space of square integrable functions. Let $T = \dfrac{d^n}{dt^n}$ and let $A : W_2^n \to Z = Z^N$ be the operator-trace of the function,

$$Au = \big(u(t_1), u(t_2), \ldots, u(t_N)\big).$$

Let

$$C = \Big\{\sigma \in W_2^m[a,b] : \frac{d^m\sigma}{dt^m} \geqslant 0\Big\},$$

the subset of $m-$ convex functions in X, where $m \leqslant n$.

Lemma 10.

(1) *A and T are linear bounded operators.*

(2) *C is a closed convex subset of X.*

(3) *If the number of the knots N is greater or equal to the order of the differentiation n, then*

$$\ker\Big\{\frac{d^n}{dt^n}\Big\} \cap \ker A = 0_X,$$

and $\ker T + \ker A$ *is closed in* X.

Proof: To prove (3) note $\ker \dfrac{d^n}{dt^n} = \Big\{x : \dfrac{d^n x}{dt^n} = 0\Big\}$ consists of polynomials of order smaller then n; while $\ker A = \{u : u(t_i) = 0, i = 1, 2, \ldots, N\}$ contains functions with zeros at these N points. The intersection of these kernels is empty, because a polynomial of degree smaller than n cannot have $N > n - 1$ zeros.

Obviously $\ker T$ and $\ker A$ are closed, their sum is also closed. □

Lemma 10 and Theorem 3 give the following result.

Theorem 4. *The problem*

$$\phi_\alpha(\sigma_*) = \min_{\sigma\in C} : \Big\{\phi(\sigma) = \alpha\Big\|\frac{d^n\sigma}{dt^n}\Big\|^2_{L_2} + \sum_{i=1}^{N}(\sigma(t_i) - z_i)^2\Big\} \tag{20}$$

has unique solution σ_* for $N \geqslant n$. When $\sigma^{(m)} \geqslant 0$,

$$\sum_{i=1}^{N}(z_i - \sigma_*(t_i))\sigma(t_i) \leqslant \alpha \int \sigma^{(n)}(t)\sigma_*^{(n)}(t)dt,$$

with equality only for the solution $\sigma_*(t)$.

PROOF: The problem has unique solution by the previous results. The condition (9) in this case is

$$-\alpha\Big(\frac{d^n}{dt^n}\Big)^*\Big(\frac{d^n\sigma_*}{dt^n}\Big)+\sum_{i=1}^{n}\big(z_i-\sigma_*(t_i)\big)k_i\in C^0.$$

From (11) it follows, that for all σ with $\sigma^{(m)}\geqslant 0$ it must be performed

$$\sum_{i=1}^{N}\big(z_i-\sigma_*(t_i)\big)\sigma(t_i)\leqslant\alpha\int\frac{d^n\sigma_*}{dt^n}\frac{d^n\sigma}{dt^n}dt.$$

Equality is acheived only for the solution $\sigma=\sigma_*$

$$\alpha\|\sigma_*^{(n)}\|^2_{L^2}=\sum\big(z_i-\sigma_*(t_i)\big)\sigma_*(t_i).$$

In fact this equality is equivalent to the condition (10). ∎

For $T=\dfrac{d^n}{dt^n}$ it is known, that

$$G_+(x-t)=\frac{(x-t)_+^{n-1}}{(n-1)!}.$$

A basis for $\ker T$ is $\{1,t,t^2,\dots,t^{n-1}\}$, and therefore $\dim\ker T=q=n$. Then

$$h_i=\sum_{j=1}^{N}h_{ij}k_j,$$

so that $(h_i,t^k)=0, i=1,2,\dots,N-n, k=0,1,\dots,n-1$. It follows, that

$$\sum_{j=1}^{N}h_{ij}t_j^k=0, i=1,2,\dots,N-n, k=0,1,\dots,n-1.$$

We have

$$f_i(t)=\left(\sum_{j=1}^{N}h_{ij}k_j(x),\frac{(x-t)_+^{n-1}}{(n-1)!}\right)=\sum_{j=1}^{N}h_{ij}\frac{(t_j-t)_+^{n-1}}{(n-1)!}, i=1,2,\dots,N-n.$$

By Theorem 3 the solution of (20) has the representation

$$\sigma_*^{(n)}(t)=x_0^{(n)}+\sum\lambda_i\sum\frac{h_{ij}(t_j-t)_+^{n-1}}{(n-1)!}=x_0^{(n)}+\sum r_j\frac{(t_j-t)_+^{n-1}}{(n-1)!},$$

where the condition $rB=0$ is equivalent to

$$\sum_{j=1}^{N}r_jt_j^{k-1}=0, k=1,2,\dots,n. \qquad (21)$$

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On integrating n times,

$$\sigma_*(t) = x_0(t) + \sum_{j=1}^{N} r_j \frac{(t_j - t)_+^{2n-1}}{(2n-1)!} + \sum_{k=0}^{n-1} c_k t^k.$$

The function

$$s(t) = \sum_{j=1}^{N} r_j \frac{(t_j - t)_+^{2n-1}}{(2n-1)!} + \sum_{k=0}^{n-1} c_k t^k$$

under the constraints (21) is a natural spline ([**1**]) of degree $2n-1$ with knots $t_1, t_2, \ldots, t_N$. Since the restriction of $s(t)$ over $(-\infty, a = t_1)$ and $(t_N = b, \infty)$ is the polynomial $\sum c_k t^k$ of degree $n-1$, we have the following result.

Theorem 5. *The solution of the problem* (20) *is a sum of a function $x_0(t)$ with zero-crossings $t_1, t_2, \ldots, t_N$ and a natural spline $s(t)$ of degree $2n-1$ with knots in these points.*

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