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ON A METHOD OF SOLVING A SMOOTHING PROBLEM

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Abstract. In the paper a function is approximated by its values in grid knots measured with errors. The problem is equivalent to the minimization of a smoothing functional under inequality constraints in Sobolev spaces. Solving the problem is reduced to solving an auxiliary problem. It is proved that the solution of the auxiliary problem is a natural spline, which under certain conditions coincides with the solution of the initial problem.

Key words: natural spline, smoothing problem, smoothing parameters, auxiliary problem, connection equation.

1. INTRODUCTION

Let $\triangle_n : a \leq t_1 < t_2 < \ldots < t_n \leq b$ be a given partition of the interval $[a, b]$, $n > 2$, where the measurements z_i of a function g at the knots t_i of $\triangle_n$ are known with some errors

$$|g(t_i) - z_i| \leq \varepsilon_i, \qquad i = 1, \ldots, n.$$

We are looking for the smoothest function, the values of which in the grid knots t_i differ from the given values z_i by no more than the values of errors $\varepsilon_i \geq 0,\ i = 1, \ldots, n$.

Let $q \geq 1$ be a given natural number. Define two functionals: the smoothing functional

$$J(f) = \int_a^b (f^{(q)}(t))^2 \, dt$$

and the functional of deviation

$$R_i(f) = (f(t_i) - z_i)^2, \qquad i = 1, \ldots, n.$$

We formulate the problem

$$J(f) \longrightarrow \min, \tag{1'}$$
$$f \in \mathbf{W}_2^q[a,b],$$
$$R_i(f) \le \varepsilon_i^2, \qquad i = 1, \dots, n, \tag{2'}$$

where $\mathbf{W}_2^q[a,b]$ is the Sobolev space of functions f with $f^{(r)}$ absolutely continuous, $r < q$, and $f^{(q)} \in \mathbf{L}_2\,[a,b]$. This is a problem of conditional minimization of the smoothing functional in the Sobolev space with constraints of inequality type on the functional $R_i(f)$. In the present paper the existence and uniqueness of the solution of the problem (1′)–(2′) will be discussed.

If $n \le q$, then the solution of the problem (1′)–(2′) is any polynomial P of degree $(q-1)$, which satisfies the conditions $P(t_i) = z_i,\ i = 1, \dots, n$. Therefore in this case there exist infinitely many solutions of the problem (1′)–(2′).

If $n > q$ and not any algebraic polynomial of degree $(q-1)$ satisfies the conditions (2′), then there exists a unique solution of the problem (1′)–(2′). This solution is the natural spline of degree $(2q-1)$ and defect 1, which satisfies the constraints (2′) and minimizes the functional $J(f)$ (see e.g. [1]).

A natural spline s of degree $(2q-1)$ over the grid $\triangle_n$ is a function which satisfies the conditions:

1. s is a polynomial of degree $(q-1)$ on each $[t_i, t_{i+1}], i = 1, \dots, n$;
2. $s \in \mathbf{C}^{2q-2}[a,b]$;
3. $s^{(q)}(t) \equiv 0$, if $t \in [a, t_1] \cup [t_n, b]$.

A function s is a natural spline of degree $(2q-1)$ over the grid $\triangle_n$ if and only if it can be written as

$$s(t) = \sum_{j=0}^{q-1} a_j t^j + \sum_{j=1}^{n} b_j (t - t_j)_+^{2q-1}, \tag{3}$$

where the coefficients b_j satisfy the equalities

$$\sum_{j=1}^{n} b_j t_j^k = 0, \qquad k = 0, \dots, q-1$$

and

$$(t - t_j)_+^k = \begin{cases} (t - t_j)^k, & t \ge t_j, \\ 0, & t < t_j, \end{cases}$$

is the truncated power function.

If the spline s interpolates g in the sense $s(t_i) = g(t_i), \quad i = 1, \dots, n$, then it is called *an interpolating spline* for g. It is well known (see e.g. [1]) that the interpolating spline has the extremal property. This fact enables us to define the interpolating spline as a solution to the interpolating problem – the problem (1′)–(2′) in the case $R_i(f) = 0, \ i = 1, \dots, n$, i.e. when $\varepsilon_i = 0, i = 1, \dots, n$,

$$J(f) \longrightarrow \min,$$
$$f \in \mathbf{W}_2^q[a,b],$$
$$f(t_i) = z_i, \qquad i = 1, \dots, n.$$

If there exist positive values among $\varepsilon_i, i = 1, \dots, n$, then the solution of (1′)–(2′) is called *a smoothing spline*.

We denote $I = \{1, \dots, n\}, I_0 = \{i \in I \mid \varepsilon_i = 0\}$ and $I_1 = \{i \in I \mid \varepsilon_i > 0\}$, i.e. $I = I_0 \cup I_1$ (the sets I_0 and I_1 can be empty).

In that case we can rewrite (1′)–(2′) in the form

$$J(f) \longrightarrow \min, \tag{1}$$
$$f \in \mathbf{W}_2^q[a,b],$$
$$R_j(f) \le \varepsilon_j^2, \ j \in I_1; \ \ f(t_j) = z_j, \ j \in I_0. \tag{2}$$

Some algorithms for constructing the unknown smoothing spline are described in [2] and [3]. But the convergence of the method of coordinate-wise descent (see e.g. [2]) and of the fine method (see e.g. [3, 4]) has not been proved. Difficulties with computing the precise solution appear already in the case of a small degree ($q = 1$ and $q = 2$, i.e. when the solution is a spline of the first degree or a cubic spline, respectively). The main purpose of the present paper is to introduce a new algorithm for solving the problem (1)–(2).

2. AUXILIARY PROBLEM

Ignatov in [5] reduced the problem (1′) with constraint

$$\sum_{i=1}^{n} R_i(f) \le \varepsilon^2$$

to an auxiliary problem of unconditional minimization. Following this idea, we propose to reduce the solution of (1)–(2) to the solution of the auxiliary problem

$$F(f) = J(f) + \sum_{j \in I_1} \frac{1}{\alpha_j} R_j(f) \longrightarrow \min, \tag{4}$$

$$f \in \mathbf{W}_2^q[a,b], \tag{1}$$
$$f(t_j) = z_j, \ \ j \in I_0,$$

where $\alpha_j > 0, j \in I_1$ are the smoothing parameters.

Theorem 1. *There exists a unique natural spline of degree* $(2q-1)$, *which satisfies the conditions:*

$$\begin{cases} (-1)^q(2q-1)!\alpha_i b_i + s_\alpha(t_i) = z_i, & i \in I_1, \\ s_\alpha(t_i) = z_i, & i \in I_0, \end{cases} \tag{5}$$

(for the definition b_i *see* (3)*). It is the unique solution of the problem* (4).

Proof. The proof of the theorem is based on the fact ([6]) that any spline s and any function $f \in W_2^q[a,b]$ satisfies the equality

$$\int_a^b f^{(q)}(t)s^{(q)}(t)\,dt = (-1)^q(2q-1)!\sum_{j=1}^n b_j f(t_j). \tag{6}$$

Note that the spline s can be written as (3), where

$$\sum_{j=1}^n b_j t_j^k = 0,\ k = 0, \dots, q-1.$$

We shall show that the system

$$\begin{cases} (-1)^q(2q-1)!\alpha_i b_i + s_\alpha(t_i) = 0, & i \in I_1 \\ s_\alpha(t_i) = 0, & i \in I_0, \\ \sum_{j=1}^n b_j t_j^k = 0, & k = 0, \dots, q-1 \end{cases} \tag{7}$$

has only a trivial solution.

Let the spline s_{0_α} be an arbitrary solution of (7). By (6) it follows that

$$\int_a^b (s_{0_\alpha}^{(q)}(t))^2\,dt = (-1)^q(2q-1)!\sum_{j=1}^n b_j s_{0_\alpha}(t_j).$$

Therefore $\int_a^b (s_{0_\alpha}^{(q)}(t))^2 dt = -((2q-1)!)^2 \sum_{j\in I_1} \alpha_j b_j^2$.

The inequalities $\int_a^b (s_{0_\alpha}^{(q)}(t))^2\,dt \geq 0$ and $\alpha_j > 0, j \in I_1$ imply that $b_j = 0,\ j \in I_1$. We get the system

$$\begin{cases} s_{0_\alpha}(t_i) = 0, & i \in I_0, \\ \sum_{j\in I_0} b_j t_j^k = 0, & k = 0, \dots, q-1. \end{cases}$$

This system corresponds to the interpolating problem, and hence the unique solution of it is the spline $s_{0_\alpha}(t) \equiv 0$. Thus we have proved that the solution of (7) is trivial, therefore the unique spline s_α^* which satisfies the condition (5) is

$$\begin{cases} (-1)^q(2q-1)!\alpha_i b_i + s_\alpha^*(t_i) = z_i, & i \in I_1, \\ s_\alpha^*(t_i) = z_i, & i \in I_0. \end{cases}$$

Next let us prove that s_α^* is the unique solution of the problem (4). Let $(s_\alpha^* + h)$ be another solution of (4), i.e.

$$(s_\alpha^* + h)(t_i) = z_i, \qquad i \in I_0.$$

Here h is a function in $\mathbf{W}_2^q[a,b]$. Therefore $h(t_i) = 0,\ i \in I_0$.

If we suppose that $h(t) \not\equiv 0$, then we get $F(s_\alpha^* + h) > F(s_\alpha^*)$, since

$$\begin{aligned}
F(s_\alpha^* + h) &- F(s_\alpha^*) \\
&= \int_a^b (h^{(q)}(t))^2 dt + 2\int_a^b s_\alpha^{*(q)}(t) h^{(q)}(t) dt \\
&\quad + \sum_{j \in I_1} \frac{1}{\alpha_j} (((s_\alpha^* + h)(t_j) - z_j)^2 - (s_\alpha^*(t_j) - z_j)^2) \\
&= \int_a^b (h^{(q)}(t))^2 dt + 2(-1)^q (2q-1)! \sum_{j=1}^n b_j h(t_j) \\
&\quad + \sum_{j \in I1} \frac{1}{\alpha_j} (2(s_\alpha^*(t_j) - z_j) h(t_j) + h^2(t_j)) \\
&= \int_a^b (h^{(q)}(t))^2 dt + 2(-1)^q (2q-1)! \sum_{j \in I_1} b_j h(t_j) \\
&\quad + \sum_{j \in I_1} \frac{1}{\alpha_j} (2(-1)^{q+1} (2q-1)! \alpha_j b_j h(t_j) + h^2(t_j)) \\
&= \int_a^b (h^{(q)}(t))^2 dt + \sum_{j \in I_1} \frac{1}{\alpha_j} h^2(t_j) > 0.
\end{aligned}$$

This proves that the spline s_α^* is the unique function, which minimizes the functional $F(f)$. □

It follows from Theorem 1 that the construction of the solution of the problem (4) can be reduced to the system of linear equations (6).

3. CONNECTION EQUATION

The main result of the present paper connects the solution of the problem (1)–(2) to the solution of the problem (4). We denote

$$\alpha = (\alpha_i \mid i \in I_1); \qquad\qquad \varepsilon^2 = (\varepsilon_i^2 \mid i \in I_1);$$

$$\varphi_i(\alpha) = R_i(s_\alpha) = (s_\alpha(t_i) - z_i)^2, \quad i \in I_1; \quad \varphi(\alpha) = (\varphi_i(\alpha) \mid i \in I_1),$$

where s_α is the solution of the problem (4). We call the vector equality

$$\varphi(\alpha) = \varepsilon^2 \tag{8}$$

the connection equation. It connects the smoothing parameters α and ε of the problem (1)–(2) and (4).

Theorem 2. *If the parameters α and ε are connected by Eq.* (8), *then the spline s_α, i.e. the solution of the problem* (4), *gives the unique solution of the problem* (1)–(2).

Proof. Let f be the solution of (1)–(2). Note that the spline s_α satisfies also the conditions (2). Let us compare the values $J(f)$ and $J(s_\alpha)$.

Suppose $J(f) \le J(s_\alpha)$. Then

$$F(f) = J(f) + \sum_{j\in I_1} \frac{1}{\alpha_j} R_j(f) \le J(s_\alpha) + \sum_{j\in I_1} \frac{1}{\alpha_j}\varepsilon_j^2$$
$$= J(s_\alpha) + \sum_{j\in I_1} \frac{1}{\alpha_j}(s_\alpha(t_i) - z_i)^2 = F(s_\alpha),$$

i.e. $F(f) \le F(s_\alpha)$.

By Theorem 1 s_α is the unique solution of the problem (4), therefore $f \equiv s_\alpha$. If $f \not\equiv s_\alpha$, we get a contradiction. Thus $J(f) > J(s_\alpha)$. □

4. CASE OF PARTIAL SMOOTHING

Consider the problem (1)–(2) in the case, where the values z_i of the function g are known exactly at all points t_i, except one point t_m.

$$J(f) \longrightarrow \min, \qquad (1^0)$$
$$f \in \mathbf{W}_2^q[a,b],$$
$$R_j(f) \le \varepsilon_j^2,\ j \in I, j \ne m;\ f(t_m) = z_m. \qquad (2^0)$$

We shall call this case *partial smoothing*.

The auxiliary problem in this case will be the following

$$F(f) = J(f) + \frac{1}{\alpha_m} R_m(f) \longrightarrow \min,$$
$$f \in \mathbf{W}_2^q[a,b],$$
$$f(t_j) = z_j,\ \ j \in I, j \ne m.$$

Without the last condition our problem (1^0)–(2^0) becomes an interpolating problem. The solution of this problem $\overline{s}$ is an interpolating spline for the vector $\overline{z} = (z_j \mid j \in I, j \ne m)$. Let us denote $\varepsilon_m^* = |\overline{s}(t_m) - z_m|$. This value ε_m^* will be called the critical value of the smoothing parameter ε.

The spline $\overline{s}$ satisfies all the conditions of the problem (1^0)–(2^0) in the case $\varepsilon_m \ge \varepsilon_m^*$, and thus the spline $\overline{s}$ is the solution of this problem.

Consider the equation

$$\varphi_m(\alpha_m) = \varepsilon_m^2 \qquad (9)$$

in the case $0 < \varepsilon_m < \varepsilon_m^*$.

Theorem 3. *The function $\varphi_m(\alpha_m)$ is continuously differentiable, strictly increasing, and*

$$\lim_{\alpha_m \to 0} \varphi_m(\alpha_m) = 0, \quad \lim_{\alpha_m \to \infty} \varphi_m(\alpha_m) = (\varepsilon_m^*)^2.$$

Proof. The spline s_α can be written as (3). Its coefficients $a_0, a_1, \dots, a_{q-1}$ and $b_1, b_2, \dots, b_n$ depend on α_m.

In our case

$$\varphi_m(\alpha_m) = (s_\alpha(t_m) - z_m)^2 = ((2q-1)!)^2 \alpha_m^2 b_m^2(\alpha_m).$$

If we prove that the coefficients are continuously differentiable, then we prove that the spline s_α, and hence the function $\varphi_m(\alpha_m)$ are continuously differentiable. The coefficients of the spline will be continuously differentiable as the solution of the following system of the algebraic equations

$$\begin{cases} (-1)^q (2q-1)! \alpha_m b_m(\alpha_m) + \sum\limits_{j=0}^{q-1} a_j(\alpha_m) t_m^j \\ \qquad + \sum\limits_{j=1}^{n} b_j(\alpha_m)(t_m - t_j)_+^{2q-1} = z_m; \\ \sum\limits_{j=0}^{q-1} a_j(\alpha_m) t_i^j + \sum\limits_{j=1}^{n} b_j(\alpha_m)(t_i - t_j)_+^{2q-1} = z_i, \\ \qquad i = 1, \dots, m-1, m+1, \dots, n; \\ \sum\limits_{j=1}^{n} b_j(\alpha_m) t_j^k = 0, \quad k = 0, \dots, q-1. \end{cases} \tag{10}$$

Let us differentiate the function $\varphi_m(\alpha_m)$,

$$\frac{\partial \varphi_m(\alpha_m)}{\partial \alpha_m} = 2(s_\alpha(t_m) - z_m) \frac{\partial s_\alpha}{\partial \alpha_m}(t_m).$$

By differentiating (3), we obtain

$$\frac{\partial s_\alpha}{\partial \alpha_m}(t) = \sum_{j=0}^{q-1} \frac{\partial a_j(\alpha_m)}{\partial \alpha_m} t^j + \sum_{j=1}^{n} \frac{\partial b_j(\alpha_m)}{\partial \alpha_m}(t - t_j)_+^{2q-1},$$

where

$$\sum_{j=1}^{n} \frac{\partial b_j(\alpha_m)}{\partial \alpha_m} t_j^k = 0, \qquad k = 0, \dots, q-1.$$

Thus $\frac{\partial s_\alpha}{\partial \alpha_m}(t)$ is a natural spline. By (6) it follows that

$$\int_a^b \left(\frac{\partial^{q+1} s_\alpha}{\partial \alpha_m \partial t^q}(t) \right)^2 dt = (-1)^q (2q-1)! \sum_{j=1}^n \frac{\partial b_j(\alpha_m)}{\partial \alpha_m} \frac{\partial s_\alpha}{\partial \alpha_m}(t_j). \quad (11)$$

In order to obtain $\frac{\partial b_j(\alpha_m)}{\partial \alpha_m}$, let us differentiate each equation of the system (10).

$$\begin{cases} (-1)^q (2q-1)! \alpha_m \frac{\partial b_m(\alpha_m)}{\partial \alpha_m} + (-1)^q (2q-1)! b_m(\alpha_m) \\ \qquad + \frac{\partial s_\alpha}{\partial \alpha_m}(t_m) = 0; \\ \frac{\partial s_\alpha}{\partial \alpha_m}(t_i) = 0, \\ \qquad i = 1, \ldots, m-1, m+1, \ldots, n; \\ \sum_{j=1}^n \frac{\partial b_j(\alpha_m)}{\partial \alpha_m} t_j^k = 0, \quad k = 0, \ldots, q-1. \end{cases}$$

Therefore, taking into account (12),

$$\begin{aligned} \int_a^b \left(\frac{\partial^{q+1} s_\alpha}{\partial \alpha_m \partial t^q}(t) \right)^2 dt &= (-1)^q (2q-1)! \frac{\partial b_m(\alpha_m)}{\partial \alpha_m} \frac{\partial s_\alpha}{\partial \alpha_m}(t_m) \\ &= \frac{1}{\alpha_m} \left(-\frac{\partial s_\alpha}{\partial \alpha_m}(t_m) - (-1)^q (2q-1)! b_m \right) \times \frac{\partial s_\alpha}{\partial \alpha_m}(t_m) \\ &= \frac{1}{\alpha_m} \left(-\left(\frac{\partial s_\alpha}{\partial \alpha_m}(t_m)\right)^2 - (-1)^q (2q-1)! b_m \frac{\partial s_\alpha}{\partial \alpha_m}(t_m) \right). \end{aligned}$$

By the first equation of (10) we have

$$(-1)^q (2q-1)! b_m = -\frac{1}{\alpha_m}(s_\alpha(t_m) - z_m).$$

Hence

$$\begin{aligned} &\int_a^b \left(\frac{\partial^{q+1} s_\alpha}{\partial \alpha_m \partial t^q}(t) \right)^2 dt \\ &= \frac{1}{\alpha_m} \left(-\left(\frac{\partial s_\alpha}{\partial \alpha_m}(t_m) \right)^2 + \frac{1}{\alpha_m}(s_\alpha(t_m) - z_m) \frac{\partial s_\alpha}{\partial \alpha_m}(t_m) \right), \end{aligned}$$

and thus

$$\begin{aligned} \frac{\partial \varphi_m(\alpha_m)}{\partial \alpha_m} &= 2(s_\alpha(t_m) - z_m) \frac{\partial s_\alpha(t_m)}{\partial \alpha_m} \\ &= 2\alpha_m^2 \int_a^b \left(\frac{\partial^{q+1} s_\alpha}{\partial \alpha_m \partial t^q}(t) \right)^2 dt + 2\alpha_m \left(\frac{\partial s_\alpha}{\partial \alpha_m}(t_m) \right)^2. \end{aligned}$$

We see that $\frac{\partial\varphi_m(\alpha_m)}{\partial\alpha_m} > 0$, so the function $\varphi_m(\alpha_m)$ is strictly increasing on the interval $(0, +\infty)$.

If $\alpha_m \to 0$, then from the first equation of (10) we get

$$\lim_{\alpha_m\to 0} s_\alpha(t_m) = z_m,$$

and the solution of this system converges to the interpolating spline for the vector $z = (z_1, \dots, z_n)$. Hence

$$\lim_{\alpha_m\to 0} \varphi_m(\alpha_m) = 0.$$

If $\alpha_m \to \infty$, then the problem tends to the interpolating problem, which has the solution $\overline{s}$. Therefore

$$\lim_{\alpha_m\to \infty} \varphi_m(\alpha_m) = (\varepsilon_m^*)^2.$$

□

Corollary 4. *For* $\varepsilon_m \in (0, \varepsilon_m^*)$ *Eq.* (9) *has a unique solution.*

REFERENCES

1. Laurent, P. J. *Approximation et optimization.* Hermann, Paris, 1972.
2. Vershinin, V. V., Zav'yalov, Yu. S., and Pavlov, N. N. *Ekstremal Properties of Splines and the Smoothing Problem.* Nauka, Novosibirsk, 1988 (in Russian).
3. Pavlov, N. N. Smoothing by cubic splines and the penalty method. *Vychisl. Sistemy*, 1983, 98, 92–102 (in Russian).
4. Pavlov, N. N. Smoothing splines of first degree. *Vychisl. Sistemy*, 1985, 108, 31–36 (in Russian).
5. Ignatov, M. I. *A Metod of Construction of Smoothing Splines of One Variable.* Preprint AN SSSR, Ural'skoe otdelenie, Syktyvkar, 1988 (in Russian).
6. Malozemov, V. N. and Pevnyj, A. B. *Polinomial Splines.* Leningrad Univ., Leningrad, 1986 (in Russian).

ÜHEST LÄHTEANDMETE SILUMISE ÜLESANDE LAHENDUSMEETODIST

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On vaadeldud ülesannet, kus funktsiooni lähendatakse tema väärtuste järgi sõlmedes, kusjuures need väärtused on antud mõningase veaga. Selline ülesanne on siledusfunktsionaali tingliku minimeerimise ülesanne Sobolevi ruumis võrratuste tüüpi kitsendustega. Püstitatud ülesande lahendamine on taandatud abiülesande lahendamisele ja tõestatud, et abiülesande lahendiks on naturaalne splain, mis teatud tingimustel langeb kokku esialgse ülesande lahendiga.