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On a method of the construction of smoothing histosplines

Natalia Budkina

Department of Mathematics, University of Latvia, Zellu St. 8, LV-1002 Riga, Latvia; budkinanat@navigator.lv

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Abstract. The problem of the approximation of a given histogram by a function from Sobolev space under inequality constraints for area matching conditions is considered. The smoothing problem is reduced to the problem of linear programming with some nonlinear restrictions.

Key words: smoothing problem, histospline, simplex method.

1. INTRODUCTION

Let a mesh $\triangle_n : a = t_0 < t_1 < ... < t_n = b$ be given for the interval $[a, b]$, and let $F = \{f_1, \ldots, f_n\}$ be a corresponding histogram, i.e., f_i is the frequency for the interval $[t_{i-1}, t_i]$, where $i = 1, \ldots, n$. The mesh sizes are denoted by $h_i = t_i - t_{i-1}$.

In many practical applications it is of interest to have a function g from the Sobolev space $W_2^r[a, b]$, which satisfies the area matching conditions

$$\int\limits_{t_{i-1}}^{t_i} g(t)dt = f_i h_i,\ i = 1, \ldots, n.$$

The problem of histopolation is solvable, but not uniquely. We propose to use the smoothing functional

$$\int\limits_a^b (g^{(r)}(t))^2\ dt$$

as an objective function.

We consider a more general case of the histopolation problem because the information of the frequencies $f_i,\ i=1,\dots,n,$ which are obtained in applications as a result of measuring, experiment or preliminary calculations may be inexact. Let $\varepsilon_i \ge 0,\ i=1,\dots,n$, be given numbers. We pose the following

Problem 1.

$$\int_a^b (g^{(r)}(t))^2\,dt \longrightarrow \min_{\substack{g\in W_2^r[a,b] \\ \left|\int_{t_{i-1}}^{t_i} g(t)dt - f_i h_i\right| \le \varepsilon_i,\, i=1,\dots,n}} . \tag{1}$$

It is a problem of smoothing histopolation. If $n \le r$, then any polynomial of degree $r-1$, which satisfies the condition of histopolation, gives the solution of the problem (1). If $n > r$ and no algebraic polynomial of degree $r-1$ satisfies the inequalities $|\int_{t_{i-1}}^{t_i} g(t)dt - f_i h_i| \le \varepsilon_i,\ \ i=1,\dots,n$, then the problem (1) has the unique solution (e.g. [1]). This solution is a spline of degree $2r$ and defect 1, which minimizes the smoothing functional under restrictions. We assume in the sequel the uniqueness of the solution.

Under the assumption of the existence and uniqueness of the solution of the problem (1) it will be reduced to the problem of quadratic programming with positive semidefined matrix and obstacles of inequality type by the series of equivalent transformations. The method for finding this solution by the modification of the simplex method is described.

2. SPACE OF INTEGRAL SPLINES

In the case of exact information (i.e. $\varepsilon_i = 0$, for all i) we have a histopolation problem the solution of which is a spline s of one variable from the space of integral splines of degree $2r$ and defect 1 over the mesh $\triangle_n$ $S(\triangle_n)$ (e.g. [1]):

$$\begin{aligned} S(\triangle_n) = \quad & \{ s \in W_2^r[a,b] \ :\ \forall g \in W_2^r[a,b] \int_{t_{i-1}}^{t_i} g(t)\,dt = 0,\ i=1,\dots,n, \\ & \Longrightarrow \int_a^b g^{(r)}(t) s^{(r)}(t)\,dt = 0 \ \}. \end{aligned}$$

This spline is called histospline.

In the case of inexact information (i.e. $\varepsilon_i > 0$ for some i) the smoothing problem (1) has also the solution from the space of integral splines (see also, e.g., [1]). Its solution is a smoothing histospline.

It is known that $s \in S(\triangle_n)$ if and only if s can be written as

$$s(t)=\sum_{j=0}^{r-1}a_jt^j+\frac{(-1)^{r+1}}{(2r)!}\sum_{i=1}^{n}d_i((t-t_i)_+^{2r}-(t-t_{i-1})_+^{2r}),$$

where the coefficients d_i satisfy the equalities

$$\sum_{i=1}^{n}d_i\int_{t_{i-1}}^{t_i}t^k\,dt=0,\quad k=0,\dots,r-1.$$

The coefficients $d_i,\ i=1,\dots,n,$ characterize the derivative of order $2r$:

$$d_i=(-1)^rs^{(2r)}(t),\quad t\in[t_{i-1},t_i].$$

We need the following

Theorem 2.1 (e.g. [1]). *A spline* $s\in S(\triangle_n)$ *is the solution of Problem* 1 *if and only if it satisfies the conditions*:

- s *is a polynomial of degree* $2r$ *on each interval* $(t_{i-1},t_i),\quad i=1,\dots,n$;
- $s\in C^{2r-1}[a,b]$;
- $s^{(q)}(a)=s^{(q)}(b)=0,\quad q=r,\dots,2r-1$;
- $\left|\int_{t_{i-1}}^{t_i}s(t)dt-f_ih_i\right|\le\varepsilon_i,\quad i=1,\dots,n$;
-

$$\begin{cases} d_i=0 \quad \textit{if} \quad \left|\int_{t_{i-1}}^{t_i}s(t)dt-f_ih_i\right|<\varepsilon_i,\\ d_i\ge 0 \quad \textit{if} \quad \int_{t_{i-1}}^{t_i}s(t)dt-f_ih_i=-\varepsilon_i,\\ d_i\le 0 \quad \textit{if} \quad \int_{t_{i-1}}^{t_i}s(t)dt-f_ih_i=\varepsilon_i, \qquad \textit{for} \quad i=1,\dots,n.\end{cases} \tag{2}$$

Lemma 2.1 (e.g. [1]). *For any function* $g\in W_2^r[a,b]$ *and any spline* $s\in S(\triangle_n)$ *there holds*

$$\int_a^b g^{(r)}(t)s^{(r)}(t)dt=\sum_{i=1}^{n}d_i\int_{t_{i-1}}^{t_i}g(t)dt.$$

If we denote by $s_i \in S(\triangle_n)$ the spline which satisfies the conditions $\int_{t_{j-1}}^{t_j} s_i(t)dt = \delta_{ij}h_j, \quad i,j = 1,\ldots,n,$ where δ_{ij} is the Kronecker symbol, then $s_1,\ldots,s_n$ is a basis of the space $S(\triangle_n)$ and any spline $s \in S(\triangle_n)$ can be written in the form

$$s(t) = \sum_{i=1}^{n} y_i s_i(t), \text{ where } y_i = \frac{1}{h_i}\int\limits_{t_{i-1}}^{t_i} s(t)dt. \tag{3}$$

3. THE SMOOTHING PROBLEM AS THE PROBLEM OF QUADRATIC PROGRAMMING

Taking into account that the solution of the smoothing problem (1) is an integral spline, we can restrict the class of functions $W_2^r[a,b]$ by the space $S(\triangle_n)$ and restate Problem 1 as

Problem 2.

$$\int\limits_a^b (s^{(r)}(t))^2\, dt \longrightarrow \min_{\substack{s\in S(\triangle_n)\\ \left|\int\limits_{t_{i-1}}^{t_i} s(t)dt - f_i h_i\right| \le \varepsilon_i,\quad i=1,\ldots,n}}.$$

This is a minimization problem in the space $S(\triangle_n)$ of dimension n. We rewrite the smoothing functional as a function of new n non-negative variables

$$z_i = \frac{1}{h_i}\int\limits_{t_{i-1}}^{t_i} s(t)dt - \left(f_i - \frac{\varepsilon_i}{h_i}\right), \qquad i = 1,\ldots,n. \tag{4}$$

Let us express the spline s with respect to z using (3) and (4):

$$s(t) = \sum_{i=1}^{n}\left(f_i - \frac{\varepsilon_i}{h_i} + z_i\right) s_i(t).$$

Therefore

$$d_i = \sum_{j=1}^{n}\left(f_j - \frac{\varepsilon_j}{h_j} + z_j\right) d_{ji}, \quad i = 1,\ldots,n, \tag{5}$$

where $(d_{ij})_{j=1,\ldots,n}$ are the coefficients of the basis spline s_i.

By Lemma 2.1 we obtain

$$
\begin{aligned}
\int\limits_a^b (s^{(r)}(t))^2 dt &= \sum_{i=1}^n d_i \int\limits_{t_{i-1}}^{t_i} s(t)dt \\
&= \sum_{i=1}^n \sum_{j=1}^n \left(f_j - \frac{\varepsilon_j}{h_j} + z_j \right) (f_i h_i - \varepsilon_i + z_i h_i) d_{ji} \\
&= \sum_{i=1}^n \sum_{j=1}^n z_i h_i z_j d_{ji} + \sum_{i=1}^n \sum_{j=1}^n z_i \left(f_j - \frac{\varepsilon_j}{h_j} \right) (h_i + h_j) d_{ji} \\
&\quad + \sum_{i=1}^n \sum_{j=1}^n \left(f_j - \frac{\varepsilon_j}{h_j} \right) (f_i h_i - \varepsilon_i) d_{ji}.
\end{aligned}
$$

By introducing the matrix $D = (h_i d_{ji})_{i,j=1,\ldots,n}$ and the vectors $c = (c_i)_{i=1,\ldots,n}$, where $c_i = \sum_{i=1}^n \sum_{j=1}^n (f_j - \varepsilon_j/h_j)(h_i d_{ji} + h_j d_{ij})$ and $z = (z_i)_{i=1,\ldots,n}$ Problem 2 can be rewritten in the matrix form:

Problem 3.

$$
zDz^T + cz^T \longrightarrow \min_{z \in I\!R^n_+,\ z_j \le 2\frac{\varepsilon_j}{h_j},\ j=1,\ldots,n}.
$$

Problem 3 is a problem of quadratic programming under linear restrictions and it is equivalent to the smoothing problem (1).

Lemma 3.1. *The matrix D is symmetric and positive semidefinite.*

Proof. The transformations of the expressions for $d_{ij} = d_j(s_i)$ and $d_{ji} = d_i(s_j)$ on the basis of Lemma 2.1

$$
h_i d_{ji} = \sum_{k=1}^n d_k(s_j) \int\limits_{t_{k-1}}^{t_k} s_i(t)dt = \int\limits_a^b s_i^{(r)}(t) s_j^{(r)}(t)dt,
$$

$$
h_j d_{ij} = \sum_{k=1}^n d_k(s_i) \int\limits_{t_{k-1}}^{t_k} s_j(t)dt = \int\limits_a^b s_i^{(r)}(t) s_j^{(r)}(t)dt
$$

prove the equality $h_i d_{ji} = h_j d_{ij}$.

The inequality $zDz^T \ge 0$ for any vector $z \in I\!R^n$ is proved by the identity

$$
zDz^T = \int\limits_a^b (s_z^{(r)}(t))^2 dt, \tag{6}
$$

where s_z is the spline which satisfies the conditions $\int_{t_{k-1}}^{t_k} s_z(t)dt = z_k h_k,\ k = 1, \ldots, n$. The equality (6) is obtained by direct calculations

$$zDz^T = \sum_{i=1}^{n} z_i h_i \sum_{j=1}^{n} z_j d_{ji} = \sum_{i=1}^{n} z_i h_i d_i(s_z) = \sum_{i=1}^{n} d_i(s_z) \int\limits_{t_{i-1}}^{t_i} s_z(t)dt$$
$$= \int\limits_a^b (s_z^{(r)}(t))^2 dt.$$

4. THE SMOOTHING PROBLEM AS THE PROBLEM OF LINEAR PROGRAMMING UNDER SOME NONLINEAR CONDITIONS

Problem 3 is a problem of quadratic programming under linear restrictions and we use Wolfe's method to reduce it to the problem of linear programming with some nonlinear conditions. The reasoning in this reduction is similar to that of [2] and we consider only important steps.

We start with the Lagrange function

$$F(z, \lambda) = zDz^\top + cz^\top + \lambda(z - 2\varepsilon)^T,$$

where $\lambda = (\lambda_i)_{i=1,\ldots,n}$ is the vector of Lagrange multipliers and $\varepsilon = (\varepsilon_i/h_i)_{i=1,\ldots,n}$.

Taking into account necessary conditions for z to be a solution of Problem 3 (e.g. [3]), by introducing slack non-negative variables $(\bar{z}_i)_{i=1,\ldots,n}$ and $(\mu_i)_{i=1,\ldots,n}$ as $\mu_i = 2(Dz^T)_i + c_i + \lambda_i$ and $\bar{z}_i = 2\varepsilon_i/h_i - z_i,\ i = 1, \ldots, n,$ we can rewrite Problem 3 as a linear programming minimization problem of an auxiliary non-negative variable u under some nonlinear restrictions:

Problem 4.

$$u \longrightarrow \min \tag{7}$$
$$2Dz^T + c^T + \lambda^T - \mu^T + uE = 0,$$
$$z + \bar{z} = 2\varepsilon,\ \mu z^T = 0,\ \lambda \bar{z}^T = 0,$$
$$z \geq 0,\ \bar{z} \geq 0,\ \lambda \geq 0, \mu \geq 0,\ u \geq 0,$$

where the vector E is any vector with components as 0, 1, and -1. The existence of a non-negative solution of Problem 3 implies that zero is the solution of Problem 4.

Theorem 4.1. *Let Problem* 1 *have the unique solution. Then it is equivalent to Problem* 4 *in the following sense*:

- *Problem* 4 *has the unique solution too,*

- *the solution of Problem* 1 *determines the solution of Problem* 4 *and the solution of Problem* 4 *determines the solution of Problem* 1 *by* (4).

The proof is similar to the proof of Theorem 3.1 from [2] and is based on the checking of the conditions (2) for the solution of (1), which are obtained by the solution z of Problem 4.

5. CONSTRUCTION BY A MODIFICATION OF THE SIMPLEX METHOD

Problem 4 differs from problems of linear programming in two simple nonlinear conditions $\mu z^\top = 0$, $\lambda(\bar{z})^\top = 0$. For the solution of the problem a modification of the simplex method based on Wolfe's and Daugavet's works [4]) is suggested. We give a short description of this algorithm.

Initial plan

- We choose any combination of z and $\bar{z}$ taking into account the condition $z^T + \bar{z}^T = 2\,\varepsilon$ and $z_i \bar{z}_i = 0,\ i = 1, \ldots, n$, (only for the initial plan) (for example, $z_i = 2\varepsilon_i / h_i,\ \bar{z}_i = 0,\ i = 1, \ldots, n$).

- The corresponding elements of μ and λ are determined in such a way that $\mu z^T = 0,\ \lambda \bar{z}^T = 0$ (for example, if $z_i = 2\varepsilon_i / h_i$, then $\mu_i = 0$).

- We take an initial value of $u > 0$, choose the sign before u (the vector E) and the corresponding $\lambda \geq 0,\ \mu \geq 0$ in such a way that they satisfy the equations $2Dz^T + c^T + \lambda^T - \mu^T + uE = 0$ (for example, if $z_i = 2\varepsilon_i / h_i,\ i = 1, \ldots, n$, then $\mu_i = 0,\ i = 1, \ldots, n$, we can take $u = \max\{|(2Dz^T + c^T)_i| :\ 1 \leq i \leq n\}$, elements of E as -1 and choose $\lambda_i = -2(Dz^T)_i - c_i + u,\ i = 1, \ldots, n$).

Iterations

Every step of the method is a transformation of the simplex table, taking into account the lexicographic ordering (it allows us to avoid iterative loops) and the additional conditions $\mu z^\top = 0$, $\lambda \bar{z}^T = 0$. We can show that the additional nonlinear condition does not prevent us from doing it by analogy of the proof of this fact for a similar system in [5], where under the assumption that the next simplex iteration cannot be done without violation of these nonlinear conditions we proved that in this case the last basic solution gives $u = 0$, i.e. the solution of (7).

There are three possibilities of the location of z_i and $\bar{z}_i$ in the table:

- z_i being in the upper part of the table means that the solution s of Problem 1 satisfies the condition $\int_{t_{i-1}}^{t_i} s(t)dt = f_i h_i + \varepsilon_i$;

- $\bar{z}_i$ being in the upper part of the table means that s satisfies the condition $\int_{t_{i-1}}^{t_i} s(t)dt = f_i h_i - \varepsilon_i$;
- location of z_i and $\bar{z}_i$ in the lower part means that s satisfies the strict inequality $|\int_{t_{i-1}}^{t_i} s(t)dt - f_i h_i| < \varepsilon_i$.

Note that z_i and $\bar{z}_i$ cannot be in the upper part of the table simultaneously.

The algorithm completes its work when the variable u appears in the upper part of the table. As was proved by Daugavet ([4]), this occurs in a finite number of steps when the matrix D is positive semidefinite.

This method give us the values of the components of the vector $(f_i - \varepsilon_i/h_i + z_i)_{i=1,\dots,n}$. The corresponding histospline can be constructed by some of the known methods of the construction of histosplines.

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Ühest siluvate histosplainide leidmise meetodist

Natalia Budkina

Töös käsitletakse antud histogrammi põhjal lähendava funktsiooni leidmist, mis määratakse kui minimiseerimisülesande lahend. Selles ülesandes on lubatavaks hulgaks Sobolevi ruumi osahulk, millesse kuuluvad funktsioonide keskmised võivad erineda histogrammi keskmistest etteantud vigade piirides, sihifunktsioon on aga loomulik norm Sobolevi ruumi elementide kõrgeimat järku tuletisest. Kasutades asjaolu, et taolise ülesande lahendiks on teadaolevalt paarisjärku naturaalsplain, näidatakse, kuidas silumisülesanne taandub ruutplaneerimise ülesandele. Saadud ruutplaneerimise ülesande omadused võimaldavad selle omakorda taandada lineaarse sihifunktsiooniga minimiseerimisülesandele, milles mittelineaarsus esineb kitsendustes. Vaatamata kitsendustes olevale mittelinaarsusele, on rakendatav simpleksmeetodi modifikatsioon, mis annab lõpliku arvu sammudega lahendi.