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On the Characterization of Non-negative Volume-Matching Surface Splines

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In this paper we study the surface spline which minimizes the Dirichlet Integral over a two-dimensional bounded domain, among all non-negative functions satisfying a finite number of volume-matching constraints. Existence and uniqueness of this surface spline are proved. A characterization by a variational inequality is given, revealing local and boundary behaviour of the surface spline. This characterization is of importance in the construction of numerical algorithms for the production of non-negative smooth surfaces from aggregated data. © 1987 Academic Press, Inc.

1. INTRODUCTION

In this paper we study the surface spline defined as the solution of the variational problem:

$$\underset{u \in H^1(\Omega)}{\text{minimize}}\ J_1(u) = \int_\Omega (u_x^2 + u_y^2)\, dx\, dy \tag{1a}$$

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subject to:

$$\int_\Omega uf_i = \alpha_i, \qquad i = 1, ..., s, \tag{1b}$$

$$u \geqslant 0 \qquad \text{a.e. in } \Omega, \qquad (1c)^1$$

where Ω is a smooth bounded region in R^2, $f_i \in L^2(\Omega)$, $i = 1, ..., s$, and $H^l(\Omega)$ is the (first Sobolev) space of functions, which together with their first-order distributional derivatives belong to $L^2(\Omega)$.

This variational approach provides a method for the production of smooth non-negative surfaces fitting a set of aggregated data of the type (1b), and, in particular, for the estimation of a density from its given volumes

$$\int_{\Omega_i} u = \alpha_i, \qquad i = 1, ..., s, \qquad (1b)'$$

over a partition $\Omega_1, ..., \Omega_s$ of the domain Ω (Tobler [10]).

The variational approach to the interpolation of function values given on a set of scattered points is well established for $\Omega = R^2$ (See, e.g., Duchon [3] and Meinguet [9]). The required surface fits the data and minimizes a roughness criterion of the form

$$J_m(u) = \int_\Omega \sum_{i=0}^{m} \binom{m}{i} \left(\frac{\partial^m u}{\partial x^i \, y^{m-i}} \right)^2, \qquad m \geqslant 2,$$

which is rotation invariant.

The same approach in case of aggregated data is studied in Dyn and Wahba [4] and Wahba [12]. For this type of data the roughness criterion $J_1(u)$ can also be considered and provides the surface spline of lowest order. In the present work we impose the additional constraint of the positivity of the surface and investigate the solution of the resulting variational problem (1), or (1) with J_1 replaced by J_m, $m \geqslant 2$.

The surface spline solving (1) (denoted hereafter by SS(1)), generalizes the notion of the univariate shape preserving algebraic spline defined by an analogous variational problem (See, e.g., Laurent [8] and Utreras [11]).

It is worth noting that problem (1), without the linear constraints (1b) (which provide the main information about the estimated function), and for $H^l(\Omega)$ replaced by $H_0^l(\Omega)$ is the well-known stationary obstacle problem in mechanics (Glowinski [6]).

[1] In case Ω is a bounded domain, the non-negativity almost everywhere in (1c) is equivalent to the non-negativity in Ω in the sense of $H^l(\Omega)$ ($u \geqslant 0$ in Ω in the sense of $H^l(\Omega)$), if $\exists \{\phi_n\} \subset C^1(\bar{\Omega})$, $\phi_n \geqslant 0$ in Ω, such that $\phi_n \to \phi$ in $H^l(\Omega)$. (See, e.g., Kinderlehrer and Stampacchia [7].)

In the following, we limit the discussion to sets of constraints (1b) satisfied by at least one smooth non-negative function. This is always the case for constraints of the form (1b)′ with $\alpha_i > 0$, $i = 1,..., s$.

In Section 2, we give a simple existence and uniqueness proof for the solution of (1). Using results from optimization theory in Banach spaces, we give in Section 3 a characterization of the SS(1) in terms of a variational inequality. In Section 4, we combine the results of Section 2 and Section 3 with a theorem of Brezis [2] to study local properties of the SS(1). In particular the SS(1) is found to be continuous and therefore non-negative everywhere in Ω, two properties which are essential for applications.

These characterizations of the solution to (1) are of crucial importance in the construction of numerical procedures for the computation of the solution, and in establishing their convergence rates (Wong [13]). The analogous characterizations of the solution to the obstacle problem (1a)+(1c) are the basis to several numerical procedures for the computation of this solution (see Glowinski [6] for a review of these methods).

We conclude by considering in Section 5 surface splines of higher order defined by similar minimization problems to (1), but with the functional in (1a) replaced by $J_m(u)$.

The results obtained are analogous to those for the case $m = 1$, with the exception of the local and boundary behaviour deduced from Brezis's result for $m = 1$.

This problem with $m \geqslant 2$ is of interest in the production of highly smooth positive surfaces fitting given aggregated data.

2. Existence and Uniqueness

THEOREM 1. *There exists a unique solution to problem* (1) *whenever* $\sum_{i=1}^{s} (\int_\Omega f_i)^2 > 0$.

Proof. Without loss of generality assume $\int_\Omega f_1 = G_1 \neq 0$, and let $\tilde{u} = u - 1/G_1 \alpha_1$. Then (1) is equivalent to

$$\min J(\tilde{u}) = \int_\Omega \tilde{u}_x^2 + \tilde{u}_y^2 \tag{2a}$$

subject to $\tilde{u} \in \tilde{H}^1(\Omega) = \{u \in H^1(\Omega) \mid \int_\Omega u f_1 = 0\}$ and

$$\int_\Omega f_i \tilde{u} = \alpha_i - \frac{G_i}{G_1} \alpha_1 \qquad \text{where} \quad G_i = \int_\Omega f_i,\ i = 2,..., s \tag{2b}$$

$$\tilde{u} \geqslant -\frac{\alpha_1}{G_1} \qquad \text{a.e. in } \Omega \tag{2c}$$

Now functions satisfying (2b) and (2c) are easily seen to form a closed convex set in $\tilde{H}^l(\Omega)$. It is also easy to see that $(J_1(u))^{1/2}$ is a norm in $\tilde{H}^l(\Omega)$. This norm is in fact equivalent to the Sobolev norm in $H^l(\Omega)$: $\|u\|^2 = J(u) + \int_\Omega u^2$ restricted to $\tilde{H}^l(\Omega)$. To prove this, it is enough to show that if $u \in \tilde{H}^l(\Omega)$, then $(\int_\Omega u)^2 \leqslant c J_1(u)$ for some $c > 0$, since by the classical inequality of Poincaré, there exists constants $c_1, c_2 > 0$ such that for any $v \in H^l(\Omega)$,

$$\int_\Omega v^2 < c_1 \int_\Omega (v_x^2 + v_y^2) + c_2 \left(\int_\Omega v\right)^2.$$

Now let $\hat{u} = u - (1/G) \int_\Omega u$, where $G = \int_\Omega 1$. Then by the above inequality

$$\int_\Omega \hat{u}^2 \leqslant c_1 J_1(\hat{u}) = c_1 J_1(u).$$

On the other hand, since $u \in \tilde{H}^l(\Omega)$, we must have

$$0 = \int_\Omega f_1 u = \int_\Omega f_1 \hat{u} + \left(\int_\Omega u\right) \frac{G_1}{G}$$

Hence $\int_\Omega u = (G/G_1) \int_\Omega f_1 \hat{u}$, and

$$\left(\int_\Omega u\right)^2 \leqslant \frac{G^2}{G_1^2} \left(\int_\Omega f_1^2\right)\left(\int_\Omega \hat{u}^2\right) \leqslant \frac{c_1 G^2}{G_1^2} \left(\int_\Omega f_1^2\right) J_1(u).$$

Thus (2) is the problem of finding the minimum norm element of a (nonempty) closed convex set in a Hilbert space, which always has a unique solution.

3. Variational Characterization

For finite dimensional optimization, the solution is usually characterized by the famous Karush-Kuhn-Tucker conditions. There are extensions of the Kuhn-Tucker theorem to Banach space setting. We will use the following extension (Girsanov [5]): If Q is a closed convex set in a Banach space H, and $J, h_1, \ldots, h_s$ are Fréchet differentiable functions on H, then a necessary condition for u to minimize $J(u)$ subjected to $u \in Q, h_i(u) = \alpha_i$, $i = 1, \ldots, s$ is that there exist multipliers $\lambda_1, \ldots, \lambda_s$, such that

$$\left(\nabla J(u) + \sum_{i=1}^{s} \lambda_i \nabla h_i(u)\right)(v - u) \geqslant 0 \qquad \forall v \in Q.$$

Furthermore, if J is convex, h_i, $i=1,\ldots,s$ are linear and there exists u^* in the interior of Q, satisfying $h_i(u^*)=\alpha_i$, $i=1,\ldots,s$, then the above condition is also sufficient for $u\in Q$ satisfying $h_i(u)=\alpha_i$, $i=1,\ldots,s$ to be the extremal solution.

To apply the above theorem to our problem, let $J(u)=a(u,u)=\int_\Omega u_x^2+u_y^2$, $h_i(u)=\int_\Omega f_i u$, $Q=\{u\in H^l(\Omega), u\geqslant 0$ a.e. in $\Omega\}$, and $H=H^l(\Omega)$. The Fréchet derivatives are given by $(\nabla J(u))(v)=2a(u,v)=2\int_\Omega (u_x v_x+u_y v_y)$ and $(\nabla h_i(u))(v)=\int_\Omega f_i v$, $i=1,\ldots,s$.

By the above result, we obtain the following characterization of the solution to (1), for any set of constraints (1b) satisfied by at least one smooth positive function:

THEOREM 2. *u is the solution to* (1) *if and only if there exist multipliers $\lambda_1,\ldots,\lambda_s$ such that*

$$a(u,v-u)\geqslant\int_\Omega f(v-u) \qquad \textit{for all} \quad v\geqslant 0, v\in H^l(\Omega) \tag{3a}$$

where $f=\sum_{i=1}^s \lambda_i f_i$

$$u\geqslant 0 \qquad \textit{a.e. in } \Omega \tag{3b}$$

$$\int_\Omega f_i u=\alpha_i, \qquad i=1,\ldots,s. \tag{3c}$$

By well-known results (see, e.g., [6] p. 4) we obtain from Theorem 2:

LEMMA 1. *Given $\lambda_1,\ldots,\lambda_s$ there is a unique function satisfying* (3a) *and* (3b). *This function minimizes $a(u,u)-\int_\Omega(\sum_{i=1}^s \lambda_i f_i)u$ among all non-negative functions in $H^l(\Omega)$.*

4. LOCAL BEHAVIOUR AND BOUNDARY CONDITIONS

If in (1), we ignore the equality and inequality constraints, then the problem becomes a classical calculus of variations problem; the local behaviour of the solution will then be given by the Euler equation (vanishing of the first variation) and the natural boundary conditions. In our problem (1), which is constrained, we expect to get a characterization of local behaviour similar to the Euler equation in the unconstrained case. We show that, roughly speaking, when the constraints are not active in a certain neighbourhood, then the solution SS(1) satisfies a differential equation locally in the neighborhood. This kind of local results are in general very difficult to prove, but our task is simplified considerably by some existing theorems on variational inequalities.

LEMMA 2. *Given $f \in L^2(\Omega)$, there exists a $\bar{u} \in H^2(\Omega)$, which is the unique solution of the following variational inequality*:

$$\int_\Omega (-\Delta\bar{u})(v-\bar{u}) \geqslant \int_\Omega f(v-\bar{u}) \qquad \textit{for all} \quad v \geqslant 0 \textit{ a.e. in } \Omega,\ v \in H^1(\Omega), \tag{4.a}$$

$$\bar{u} \geqslant 0 \qquad \textit{in } \Omega \tag{4b}$$

$$\frac{\partial \bar{u}}{\partial n} = 0 \qquad \textit{a.e.} \text{ on } \partial\Omega \tag{4c}$$

where $\Delta u = u_{xx} + u_{yy}$ is the Laplacian of u and $(\partial u/\partial n)$ is the normal derivative at the boundary $\partial\Omega$.

Proof. This is a special case of Theorem 1.12 in Brezis [2, p. 55], where we take

$$\beta(r) \equiv 0, \qquad -\infty < r < \infty,$$

in applying that theorem.

This result is related to the solution of (1) in the following:

LEMMA 3. *Let $\bar{u} \in H^2(\Omega)$ satisfy* (4). *Then $\bar{u}$ satisfies also* (3a).

Proof. Since $\bar{u} \in H^2(\Omega)$, we can use Green's fomula to write

$$\int_\Omega \bar{u}_x(v-\bar{u})_x + \bar{u}_y(v-\bar{u})_y = \int_\Omega (-\Delta\bar{u})(v-\bar{u}) + \int_{\partial\Omega} \frac{\partial\bar{u}}{\partial n}(v-\bar{u}).$$

The second integral in the right-hand side vanishes, because the function $\bar{u}$ satisfies the boundary conditions in (4). Therefore

$$a(\bar{u}, v-\bar{u}) = \int_\Omega (-\Delta\bar{u})(v-\bar{u}) \geqslant \int_\Omega f(v-\bar{u})$$
$$\text{for all } v \geqslant 0 \text{ a.e. in } \Omega,\ v \in H^1(\Omega),$$

and $\bar{u}$ satisfies (3a).

Combining the results of Theorem 2 and Lemmas 1–3, we obtain a differential type necessary and sufficient condition for u to be a solution of (1).

THEOREM 3. *u is the solution to* (1) *iff the following conditions are satisfied*:

$$u \in H^2(\Omega) \tag{5a}$$

there exist $\lambda_1,..., \lambda_s$ such that u satisfies

$$\int_\Omega (-\Delta u)(v-u) \geqslant \int_\Omega \left(\sum_{i=1}^{s} \lambda_i f_i\right)(v-u) \quad \text{for all } v \geqslant 0 \text{ a.e. in } \Omega,\ v \in H^1(\Omega) \tag{5b}$$

$$u \geqslant 0 \qquad \text{in } \Omega \tag{5c}$$

$$\frac{\partial u}{\partial n} = 0 \qquad \text{on } \partial\Omega \tag{5d}$$

$$\int_\Omega u f_i = \alpha_i, \qquad i = 1,..., s. \tag{5e}$$

Proof. The sufficiency follows from Lemma 3 and Theorem 2. To prove the necessity of these conditions assume u to be the solution of (1). Then by Theorem 2, there exist $\lambda_1,..., \lambda_s$ such that u satisfies (3a), and by Lemma 2, there exists $\bar{u} \in H^2(\Omega)$ satisfying (5b), (5c), (5d), with $\lambda_1,..., \lambda_s$ as in (3a). Hence by Lemma 3 $\bar{u}$ satisfies (3a) and (3b), which in view of Lemma 1 implies that $\bar{u}$ coincides with u. This completes the proof of the theorem.

Remark. The boundary condition (5d) is the natural condition, as in the classical variational problems with "free boundary".

Property (5b) of the solution of (1) is equivalent to the following local behaviour in the distributional sense (Brezis [2]):

$$(-\Delta u) \geqslant \sum_{i=1}^{s} \lambda_i f_i \quad \text{in } \Omega, \qquad (-\Delta u) = \sum_{i=1}^{s} \lambda_i f_i \quad \text{in } \{x \in \Omega: u(x) > 0\}. \tag{5b$'$}$$

Moreover since $u \in H^2(\Omega)$, $\Delta u \in L^2(\Omega)$, and (5b)$'$ holds almost everywhere in Ω. Thus (5b) in view of (5a) is equivalent to:

$$-\Delta u - \sum_{i=1}^{s} \lambda_i f_i \geqslant 0 \quad \text{a.e. in } \Omega, \qquad \left(-\Delta u - \sum_{i=1}^{s} \lambda_i f_i\right) u = 0 \quad \text{a.e. in } \Omega. \tag{5b*}$$

5. Surface Splines of Higher-Order

Similar analysis as done for the SS(1) can be carried over to the surface spline of order $m \geqslant 2$, SS(m), defined as the solution of the variational problem:

$$\min_{u \in H^m(\Omega)} J_m(u) = \iint_\Omega \sum_{i=0}^{m} \binom{m}{i} \left(\frac{\partial^m u}{\partial x^i\, \partial^{m-i} y}\right)^2 \tag{6a}$$

subject to

$$\int uf_i = \alpha_i, \qquad i = 1, \ldots, s \tag{6b}$$

$$u \geqslant 0 \qquad \text{in } \Omega. \tag{6c}$$

Here Ω is a smooth bounded region in R^2, $f_i \in L^2(\Omega)$, $i = 1, \ldots, s$, and $H^m(\Omega)$ is the m'th order Sobolev space

$$H^m(\Omega) = \left\{ u \;\middle|\; \frac{\partial^k u}{\partial x^i \, \partial y^{k-i}} \in L^2(\Omega),\ i = 0, \ldots, k,\ k = 0, \ldots, m \right\}.$$

For $m \geqslant 2$ all functions in $H^m(\Omega)$ are continuous on $\bar{\Omega}$, and the non-negativity in (6c) is pointwise.

For this problem we obtain analogous results to Theorems 1 and 2 for the case $m = 1$, for sets of linear constraints (6b) satisfying the following two assumptions:

(i) There exists a smooth positive function satisfying (6b).

(ii) There does not exist a polynomial q of total degree k, $k < m$, satisfying $\int_\Omega f_i q = 0$, $i = 1, \ldots, s$.

For the SS(m), existence, uniqueness, and characterization in terms of a variational inequality are derived by the same arguments used in Sections 2, 3. We formulate the results and omit the proofs.

THEOREM 4. *There exists a unique solution to problem* (6). u *is the solution to* (6) *iff there exist multipliers* $\lambda_1, \ldots, \lambda_s$ *such that*

$$a_m(u, v - u) \geqslant \int_\Omega (v - u) \sum_{i=1}^{s} \lambda_i f_i \qquad \textit{for all } v \geqslant 0,\ v \in H^m(\Omega) \tag{7a}$$

$$u \geqslant 0 \qquad \textit{in } \Omega \tag{7b}$$

$$\int_\Omega f_i u = \alpha_i, \qquad i = 1, \ldots, s. \tag{7c}$$

where

$$a_m(u, v) = \int_\Omega \sum_{i=0}^{m} \binom{m}{i} \frac{\partial^m u}{\partial x^i \, \partial y^{m-i}} \frac{\partial^m v}{\partial x^i \, \partial y^{m-i}}. \tag{8}$$

In order to conclude local and boundary behaviour of the solution to (6), an extension of Brezis's result (Lemma 2) to $m \geqslant 2$ is needed. At this stage the extension of Theorem 3 to $m \geqslant 2$ is yet a conjecture:

Conjecture. u is the solution to (6) if the following conditions are satisfied:

$$u \in H^{2m}(\Omega) \tag{9a}$$

there exist $\lambda_1, ..., \lambda_s$ such that u satisfies

$$(-1)^m \int_\Omega \Delta^m u(v-u)$$

$$\geqslant \int_\Omega \left(\sum_{i=1}^{s} \lambda_i f_i \right)(v-u) \qquad \text{for all } v \geqslant 0, v \in H^m(\Omega) \tag{9b}$$

$$u \geqslant 0 \qquad \text{in } \Omega \tag{9c}$$

$$\delta_{2m-i} u = 0 \qquad \text{on } \partial\Omega, i = 1, ..., m \tag{9d}$$

$$\int_\Omega u f_i = \alpha_i, \qquad i = 1, ..., s \tag{9e}$$

where δ_{2m-i}, $i = 1, ..., m$ are differential operators of order $2m - i$ defined by the generalizd Green formula (Aubin [1]):

$$a_m(u, v) = (-1)^m \int_\Omega (\Delta^m u) v + \sum_{i=0}^{m-1} \int_{\partial\Omega} (\delta_{2m-1-i} u) \frac{\partial^i}{\partial n^i} v. \tag{10}$$

The local behaviour of u in Ω implied by (9a) and (9b) is:

$$(-1)^m \Delta^m u \geqslant \sum_{i=1}^{s} \lambda_i f_i \qquad \text{a.e. in } \Omega \tag{11a}$$

$$\left[(-1)^m \Delta^m u - \sum_{i=1}^{s} \lambda_i f_i \right] \cdot u = 0 \qquad \text{a.e. in } \Omega. \tag{11b}$$

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