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NIRA DYN
DAVID LEVIN

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CONSTRUCTION OF SURFACE SPLINE INTERPOLANTS OF SCATTERED DATA OVER FINITE DOMAINS (*)

by Nira DYN and David LEVIN [1]

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Abstract — *A numerical method for smooth interpolation of scattered data over a finite two dimensional domain Ω is presented The interpolating function is defined by minimization of a Dirichlet-type integral of order $\geqslant 2$ over Ω, measuring the roughness of the surface The case corresponding to $\Omega = R^2$ results in the so-called « thin plate » spline A Ritz-type method for approximating the finite domain interpolating surface spline is developed, based on a set of basis functions including the fundamental « thin plate » splines Numerical experiments are appended, demonstrating the reduction of the roughness measure as compared to that of the « thin plate » spline*

Résumé — *On presente une methode numerique pour l'interpolation de donnees irregulierement réparties sur un domaine fini bidimensionnel Ω par une surface regulière La fonction d'interpolation est défínie par minimisation d'une intégrale du type de Dirichlet, d'onde $\geqslant 2$, sur Ω, qui mesure la qualité de l'approximation de la surface Le cas où $\Omega = R^2$ correspond aux splines de type « plaque mince » On élabore une methode de Ritz pour approcher la surface spline d'interpolation dans le cas d'un domaine fini, basée sur un ensemble de fonctions de base comprenant les splines fondamentales du type « plaque mince » On inclut des resultats numeriques, qui mettent en evidence la réduction du défaut d'approximation par rapport a celui de la spline du type « plaque mince »*

1. INTRODUCTION

A univariate interpolatory spline can be introduced as the solution to the problem of minimizing the quadratic seminorm

$$| u |_{[a,b],m} = \left\{ \int_a^b | u^{(m)}(t) |^2 \, dt \right\}^{1/2} \tag{1.1}$$

(*) Received in April 1981.
(1) School of Mathematical Sciences, Tel Aviv University, Ramat-Aviv, Tel Aviv, Israël

among all u, $u^{(m)} \in L_2[a, b]$, satisfying the interpolation conditions

$$u(x_i) = s_i\,, \quad i = 1, 2, \dots, N\,, \tag{1.2}$$

with $N \geqslant m \geqslant 1$ and $\{ x_i \}$ being distinct points in $[a, b]$.

This minimum principle is extended to the multivariate case as follows :

Given a domain Ω in R^n and N distinct points $\{ z_i = (x_1^{(i)}, \dots, x_n^{(i)}) \}$ in Ω, find a function $u \in H^m(\Omega)$ such that

$$u(z_i) = s_i\,, \quad 1 \leqslant i \leqslant N \tag{1.3}$$

for some prescribed reals $\{ s_i \}$, and such that $| u |_{\Omega,m}$ is minimal where

$$| u |_{\Omega,m}^2 = \sum_{i_1, i_2, \dots, i_m = 1}^{n} \int_\Omega \left| \frac{\partial^m u(x_1, \dots, x_n)}{\partial x_{i_1}\, \partial x_{i_2} \dots \partial x_{i_m}} \right|^2 dx_1 \dots dx_n\,. \tag{1.4}$$

Duchon [2] and Meingnet [4] give closed form solutions of this problem for $\Omega = R^2$ and term these solutions « thin plate » splines.

In the univariate case the solution of the problem (1.1)-(1.2) accepts the same values in the interval $[x_1, x_N]$ for any $a \leqslant x_1$ and $b \geqslant x_N$, and also in case of the seminorm (1.1) defined on R^1 :

$$| u |_{R,m} = \left\{ \int_{-\infty}^{\infty} | u^{(m)}(t) |^2\, dt \right\}^{1/2}.$$

However, this nice property does not hold in higher dimensional spaces, where the solution does depend upon the geometry of the domain Ω.

Intuitively, for given scattered data points $\{ z_i \}_{i=1}^N$ one expects to obtain a better interpolation approximation by using the seminorm (1.4) chosen over a domain which is characteristic to the distribution of the data points rather than over all R^n. The purpose of this work is to investigate the performance of a 2-dimensional surface spline interpolants based upon finite domain seminorms $| \ |_{\Omega,m}$ in comparison with the solution corresponding to $| \ |_{R^2,m}$. Using some theoretical results of Duchon [2] and Meingnet [4] on the formal representation of surface spline interpolants, a numerical procedure is suggested for approximating the solution of (1.3)-(1.4) for $n = 2$, $m \geqslant 1$ and « nice » domains Ω in R^2. Some numerical results are presented for $m = 2$ and polygonal domains, and the results are compared with those obtained by the « thin plate » splines. It is concluded that in many cases a significant improvement upon « thin plate » splines can be obtained, an improvement which justifies the extra computational effort needed for computing the surface spline interpolants over finite domains.

2. CHARACTERIZATION OF THE SURFACE SPLINE INTERPOLANTS OVER FINITE DOMAINS

Let Ω be a simply connected domain in R^2. Let $z_i = (x_1^{(i)}, x_2^{(i)}), i = 1, 2, \dots, N$ be N distinct points in Ω and let s_i, $i = 1, 2, \dots, N$ be any given data set of N real numbers. As it is done in the univariate case one wants to find a function which interpolates the given data and is smooth over Ω is some sense. As a roughness measure we use the functionals

$$J_m(u) = \int_\Omega \sum_{i=0}^{m} \binom{m}{i} \left(\frac{\partial^m u}{\partial x_1^i \, \partial x_2^{m-i}} \right)^2 dx_1 \, dx_2 \quad m \geqslant 2\,, \tag{2.1}$$

defined on the Sobolev space

$$H^m(\Omega) = \left\{ u \,\middle|\, \frac{\partial^k u}{\partial x_1^i \, \partial x_2^{k-i}} \in L^2(\Omega)\,, \quad 0 \leqslant i \leqslant k\,, k \leqslant m \right\}.$$

For $m = 2$ $J_m(u)$ is the stress energy of a plate of shape Ω under a distortion u. The surface spline interpolant is thus the solution of the problem :

$$\left. \begin{array}{l} \min\limits_{u \in H^m(\Omega)} J_m(u) \\ u(z_i) = s_i\,, \quad i = 1, 2, \dots, N\,. \end{array} \right\} \tag{2.2}$$

$J_m(u)$ is a seminorm on $H^m(\Omega)$ which can be written as

$$J_m(u) = A_m(u, u) \tag{2.3}$$

where A_m is a semi-inner-product on $H^m(\Omega)$

$$A_m(u, v) = \int_\Omega \sum_{i=0}^{m} \binom{m}{i} \left(\frac{\partial^m u}{\partial x_1^i \, \partial x_2^{m-i}} \right) \left(\frac{\partial^m v}{\partial x_1^i \, \partial x_2^{m-i}} \right) dx_1 \, dx_2 \tag{2.4}$$

for $u, v \in H^m(\Omega)$.

Since $A(u, u) = 0$ if and only if $u \in Q_m$ where

$$Q_m = \text{span} \{ x_1^i \, x_2^j \mid i + j < m \} \equiv \text{span} \{ q_1, q_2, \dots, q_M \}$$

with $M = \binom{m+1}{2}$, (2.2) has a unique solution if the matrix $\{ q_i(z_j) \}_{i=1,j=1}^{M\ \ N}$ is of degree M. We assume, without loss of generality, that $\{ q_i(z_{N-j+1}) \}_{i,j=1}^{M}$ is non-singular and denote the points $z_{N-M+1}, \dots, z_N$ by $y_1, \dots, y_M$. Under this assumption problem (2.2) for $m \geqslant 2$ has a unique solution, since

$H^m(\Omega) \subset C(\Omega)$ for $m \geq 2$ and the linear functionals $L_i f = f(z_i)$, $f \in H^m(\Omega)$, are bounded. It can be shown as in [3, 4] that this solution is of the form

$$u^* = \sum_{i=1}^{N-M} \nu_i \phi_i + \sum_{i=1}^{M} \mu_i q_i \tag{2.5}$$

where the coefficients $\{ \nu_i \}$ and $\{ \mu_i \}$ are determined by the interpolation conditions

$$u^*(z_i) = s_i, \quad i = 1, ..., N \tag{2.6}$$

and the ϕ_i, $1 \leqslant i \leqslant N - M$, are characterized variationally by

$$\begin{cases} A_m(\phi_i, f) = f(z_i) + \sum_{j=1}^{M} a_{ij} f(y_j) \quad \forall f \in H^m(\Omega) & (2.7) \\ \phi_i(y_j) = 0, \quad j = 1, ..., M. & (2.8) \end{cases}$$

In particular by taking $f \in Q_m$ in (2.7) we get

$$\sum_{j=1}^{M} a_{ij}\, q(y_j) + q(z_i) = 0 \quad \forall q \in Q_m. \tag{2.9}$$

By assumption $C = \{ q_i(y_j) \}_{i,j=1}^{M}$ is non-singular and therefore the a_{ij} in (2.7) are given by

$$(a_{i1}, a_{i2}, ..., a_{iM})^T = - C^{-1}(q_1(z_i), ..., q_M(z_i))^T. \tag{2.10}$$

Combining (2.7)-(2.9) with (2.5) and (2.6) we conclude that u^* is characterized variationally by

$$A_m(u^*, f) = \sum_{i=1}^{N} \lambda_i f(z_i), \quad f \in H^m(\Omega), \tag{2.11}$$

$$u^*(z_i) = s_i, \quad i = 1, ..., N \tag{2.12}$$

and $\lambda_1, ..., \lambda_N$ are constrained by the substitutions of $q_1, ..., q_M$ to satisfy

$$\sum_{i=1}^{N} \lambda_i q_j(z_i) = 0, \quad j = 1, ..., M. \tag{2.13}$$

In fact $\lambda_1, ..., \lambda_N$ are the Lagrange multipliers for the variational problem (2.2), that is u^* minimizes the functional

$$J_m(u) + \sum_{i=1}^{N} \lambda_i [u(z_i) - s_i]. \tag{2.14}$$

Let Ω be a « nice » domain such that the generalized Green's formula holds [1] :

$$A_m(u, v) = (-1)^m \int_\Omega (\Delta^m u)\, v\, dx_1\, dx_2 + \sum_{j=0}^{m-1} \int_\Gamma \delta_{2m-1-j}(u) \frac{\partial^j v}{\partial n^j}\, ds$$

where $\Delta = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$, δ_i is a differential operator of order i and $\partial/\partial n$ is the normal derivative at the boundary Γ of Ω. Then the variational characterization (2.11), (2.12) is equivalent to the differential characterization [1] :

$$(-1)^m (\Delta^m u^*)(z) = \sum_{i=1}^{N} \lambda_i\, \delta(z - z_i), \quad z = (x_1, x_2) \in \Omega \qquad (2.15)$$

$$\delta_{m+j}(u^*) = 0, \quad j = 0, \dots, m-1 \quad \text{on} \quad \Gamma \qquad (2.16)$$

$$u^*(z_i) = s_i, \quad i = 1, \dots, N \qquad (2.17)$$

with $\lambda_1, \dots, \lambda_N$ constants constrained by (2.13).

A fundamental solution of the operator $(-1)^m \Delta^m$, namely a function satisfying

$$(-1)^m \Delta^m \psi(z, \zeta) = \delta(z - \zeta) \qquad (2.18)$$

is known explicitly as [2, 4] :

$$\psi(z, \zeta) = C_m \mid z - \zeta \mid^{2(m-1)} \log \mid z - \zeta \mid, \quad C_m^{-1} = 2^{2m-1} \pi[(m-1)!]^2. \qquad (2.19)$$

The function $\psi(z, \zeta)$ is analogous to the univariate fundamental solution $\frac{1}{(2m-1)!}(x - \xi)_+^{2m-1}$ giving rise to the spline functions. Using the fundamental solution (2.19) we can write u^* as

$$u^*(z) = \sum_{i=1}^{N} \lambda_i\, \psi_i(z) + W(z), \qquad (2.20)$$

with $\lambda_1, \dots, \lambda_N$ constrained by (2.13), $\psi_i(z) \equiv \psi(z, z_i)$, $i = 1, \dots, N$, and $W(z) \in H^{2m}(\Omega)$ a solution of the boundary value problem

$$\Delta^m W = 0 \quad \text{in} \quad \Omega \qquad (2.21)$$

$$\delta_{m+j} W = -\delta_{m+j}\left[\sum_{i=1}^{N} \lambda_i\, \psi(z, z_i)\right], \quad j = 0, \dots, m-1, \quad \text{on} \quad \Gamma. \qquad (2.22)$$

The variational characterization of $W(z)$ in view of (2.11) and (2.20) is

$$A_m(W,f) = \sum_{i=1}^{N} \lambda_i f(z_i) - \sum_{i=1}^{N} \lambda_i A_m(\psi_i, f), \quad f \in H^m(\Omega). \tag{2.23}$$

By (2 18) and Green's formula, (2 23) is equivalent to

$$A_m(W,f) = -\sum_{j=0}^{m-1} \int_\Gamma \delta_{2m-1-j} \left[\sum_{i=1}^{N} \lambda_i \psi(z, z_i) \right] \frac{\partial^j f}{\partial n^j} ds, \quad f \in H^m(\Omega). \tag{2 24}$$

The solution to the boundary value problem (2 21)-(2 22) for given $\lambda_1, \quad , \lambda_N$ is determined uniquely up to a polynomial in Q_m Thus (2 21)-(2 22) together with the $N + M$ conditions (2 12)-(2 13) determine a unique function $W(z)$ and a set of constants $\lambda_1, \quad , \lambda_N$

In the case of the « thin plate » spline u^* is given by (2 20) with $W(z) = \sum_{i=1}^{M} \gamma_i q_i \in Q_m$, and the $N + M$ unknown $\lambda_1, \quad , \lambda_N, \gamma_1, \quad , \gamma_M$ are determined by the $N + M$ conditions (2 12)-(2 13) This leads to a linear system of order $N + M$ in the unknowns

3. APPROXIMATION OF THE SURFACE SPLINE INTERPOLANTS OVER FINITE DOMAINS

Let $\Phi = \{ q_1, \quad , q_M, \varphi_1, \varphi_2, \quad \}$ be a complete set of functions in

$$V^{2m}(\Omega) = \{ \varphi \mid \varphi \in H^{2m}(\Omega), \Delta^m \varphi = 0 \text{ in } \Omega \} \tag{3 1}$$

The solution of the boundary value problem (2 21)-(2 22) can be well approximated by a finite sum of the form

$$W_n(z) = \sum_{j=1}^{n} b_j^{(n)} \varphi_j(z) + \sum_{j=1}^{M} c_j^{(n)} q_j(z) \tag{3.2}$$

provided that n is large enough A system of $n + M$ linear equations for the coefficient $\{ b_j^{(n)} \}_{j=1}^n, \{ c_j^{(n)} \}_{j=1}^M$ is obtained, as in the Ritz method, by applying the variational characterization (2 23) to the subspace of basis functions $\{ q_1, \ldots, q_M, \varphi_1, \quad ., \varphi_n \}$ This procedure yields equations of two types :

$$\sum_{j=1}^{n} b_j^{(n)} A_m(\varphi_j, \varphi_i) - \sum_{l=1}^{N} \lambda_l^{(n)} \varphi_i(z_l) + \sum_{l=1}^{N} \lambda_l^{(n)} A_m(\psi_l, \varphi_i) = 0, \quad i = 1, \ldots, n, \tag{3.3}$$

$$\sum_{l=1}^{N} \lambda_l^{(n)} q_k(z_l) = 0, \quad k = 1, \ldots, M. \tag{3.4}$$

These equations together with the N interpolation conditions

$$\sum_{j=1}^{n} b_j^{(n)} \varphi_j(z_i) + \sum_{l=1}^{N} \lambda_l^{(n)} \psi_l(z_i) + \sum_{k=1}^{M} c_k^{(n)} q_k(z_i) = s_i , \quad i = 1, \dots, N \quad (3.5)$$

constitute a linear system of $N + M + n$ equations in the $N + M + n$ coefficients of the approximate solution of (2.11)-(2.12), given by

$$u_n = \sum_{i=1}^{N} \lambda_i^{(n)} \psi_i + \sum_{i=1}^{n} b_i^{(n)} \varphi_i + \sum_{i=1}^{M} c_i^{(n)} q_i . \quad (3.6)$$

In case n can be taken much smaller than N, the set of equations (3.3), (3.4), (3.5) differs from the set of equations for the « thin plate » splines by a small number of comparatively complicated equations, which depend on the geometry of the domain. The coefficients in these equations consist of the bi-linear forms $A_m(\varphi_i, \varphi_j)$, $A_m(\psi_l, \varphi_j)$ $i, j = 1, \dots, n$, $l = 1, \dots, N$, which in general can be evaluated only numerically. Yet by Green's formula and since $\Delta^m \varphi_i = 0$, $i = 1, \dots, n$, the area integrals defining these forms can be computed by line integrals along the boundary of the domain :

$$A_m(\varphi_i, \varphi_j) = \sum_{r=0}^{m-1} \int_\Gamma \delta_{2m-1-r}(\varphi_i) \frac{\partial^r}{\partial n^r} \varphi_j \, ds \quad (3.7)$$

$$A_m(\psi_l, \varphi_j) = \sum_{r=0}^{m-1} \int_\Gamma \delta_{2m-1-r}(\varphi_j) \frac{\partial^r}{\partial n^r} \psi_l \, ds \quad (3.8)$$

$$= \varphi_j(z_l) + \sum_{r=0}^{m-1} \int_\Gamma \delta_{2m-1-r}(\psi_l) \frac{\partial^r}{\partial n^r} \varphi_j \, ds .$$

For a « nice » finite domain Ω, where Re, Im $\{ z^j \}_{j=0}^{\infty}$ form a complete set of harmonic functions ($z = x_1 + ix_2$), the set of functions

$$\text{Re, Im} \{ \bar{z}^k z^j \}_{j=0,k=0}^{\infty \ \ m-1} \quad (3.9)$$

constitutes a complete set of m-harmonic functions. This follows from the observation that the general representation of an m-harmonic function in Ω is

$$\text{Re} \left\{ \sum_{k=0}^{m-1} \bar{z}^k f_k(z) \right\} \quad (3.10)$$

where $f_0(z), \dots, f_{m-1}(z)$ are analytic in Ω. Indeed, (3.10) is obtained recursively from the identity

$$\Delta \, \text{Re} \{ \bar{z}^k f(z) \} = 4 \, k \, \text{Re} \{ \bar{z}^{k-1} f'(z) \} , \quad (3.11)$$

and from the fact that any harmonic function is the real part of an analytic function.

In this work we present several numerical examples computed by this method for the case $m = 2$ and with the basis functions $\{ \varphi_1, \dots, \varphi_n \}$ taken from the set (3.9). Other choices of basis functions are yet to be investigated.

4. NUMERICAL EXPERIMENTS FOR THE CASE $m = 2$

In this section we discuss the application of the method of section 3 in the case $m = 2$, which is analogous to the univariate cubic spline. For this case the extra computational work in the evaluation of the coefficients in the n equations (3.3) is still reasonable. We present several examples indicating that this additional effort is worthwhile.

We have produced a program for calculating the approximation u_n ((3.6)) over polygonal domains using the following basis functions :

$$\left.\begin{aligned} \varphi_1 &= \operatorname{Re}(\bar{z}z) \\ \varphi_{2+4j} &= \operatorname{Im}(z^{j+2}) \\ \varphi_{3+4j} &= \operatorname{Re}(z^{j+2}) \\ \varphi_{4+4j} &= \operatorname{Im}(\bar{z}z^{j+2}) \\ \varphi_{5+4j} &= \operatorname{Re}(\bar{z}z^{j+2}) \end{aligned}\right\} \quad j \geqslant 0 \tag{4.1}$$

where $z = x_1 + ix_2$. The formulae (3.7), (3.8) do not hold for non-smooth domains, therefore, we compute the coefficients in equations (3.3) by using the following version of Green's formula :

$$A_2(u, v) = \int_\Omega (\Delta^2 u)\, v\, dx_1\, dx_2 - \int_\Gamma \left(\frac{\partial}{\partial n} \Delta u\right) v\, ds + \int_\Gamma \nabla \frac{\partial u}{\partial n} \cdot \nabla v\, ds\,. \tag{4.2}$$

With this formula the various bilinear forms in (3.3) as well as the roughness measure $J_2(u_n)$ can be evaluated by line integrals. The actual numerical computation of the line integrals has been carried out by using Simpson rule.

In the following table we demonstrate the reduction in the roughness measure $J_2(u_n)$ as n increases, for various data sets over the L-shaped domain :

$$\Omega = \{ (x_1, x_2) \mid -0.5 \leqslant x_1, x_2 \leqslant 0.5, x_1 \geqslant 0 \quad \text{or} \quad x_2 \geqslant 0 \}\,. \tag{4.3}$$

The interpolation points are chosen randomly in Ω and the data is taken from the test functions :

$$\begin{aligned} f_1 &= 4\, x_1\, x_2 \\ f_2 &= \sin(10\, x_1\, x_2) \\ f_3 &= \exp(-25(x_1^2 + x_2^2 - 0.1)^2)\,. \end{aligned}$$

The upper index in $J_2^N(u_n)$ indicates the number of data points

	f_1	f_2	f_3
$J_2^{13}(u_0)$	25 0	98 0	85 0
$J_2^{13}(u_7)$	17 4	76 0	78 0
$J_2^{13}(u_{15})$	16 6	72 0	74 0
$J_2^{27}(u_0)$	28 1	105 0	132 0
$J_2^{27}(u_7)$	19 0	87 0	124 0
$J_2^{27}(u_{15})$	18 3	82 0	119 0

For the cases tested the sequence $\{ J_2(u_n) \}$ seems to be converging The reduction in the roughness measure of u_n with increasing n from that of the « thin plate » spline u_0 is also reflected in the pointwise approximation to the test functions It turns out that the oscillations of the approximation are significantly reduced in a sub-region of Ω which is not too close to Γ However, as we get closer to the boundary of Ω the approximation u_n is sometimes even worse than u_0 We believe that this is due to the enforcement of the so-called « natural boundary conditions » (2 16) which are in fact unnatural to the functions tested

As a result of our numerical experiments we conclude that for a smooth interpolation to a given data over Ω one should solve the problem (2 2) over a somewhat larger domain $\Omega \supset \Omega$ For a suitable chosen Ω one would get an optimal trade-off between the reduction of the roughness measure and the intrusion of the natural boundary conditions Further results in this direction are yet under investigation

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