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Interpolation by Regularized Spline with Tension: I. Theory and Implementation[1]

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Bivariate and trivariate functions for interpolation from scattered data are derived. They are constructed by explicit minimization of a general smoothness functional, and they include a tension parameter that controls the character of the interpolation function (e.g., for bivariate case the surface can be tuned from a "membrane" to a "thin steel plate"). Tension can be applied also in a chosen direction, for modeling of phenomena with a simple type of anisotropy. The functions have regular derivatives of all orders everywhere. This makes them suitable for analysis of surface geometry and for direct application in models where derivatives are necessary. For processing of large datasets (thousands of data points), which are now common in geosciences, a segmentation algorithm with a flexible size of overlapping neighborhood is presented. Simple examples demonstrating flexibility and accuracy of the functions are presented.

KEY WORDS: surface modeling, scattered data interpolation, segmented processing.

INTRODUCTION

In spite of a large number of available interpolation methods and computer software for surface modeling, the task of surface computation from scattered data can often be time consuming and difficult. Major problems are connected with processing of large datasets (100,000 data points are now common in terrain modeling) and with interpolation from data with strongly nonhomogeneous spatial distribution as is the case with digitized contours or clustered data (e.g., resulting from processing of geological drill-hole measurements). Moreover, a growing need exists not only for interpolation but also for an analysis of modeled surfaces. With the move from lumped hydrological, geomorphological, and related models to spatially distributed ones, topographic parameters computed

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for dense grids are necessary (Moore et al., 1991). Many traditional methods are not sufficient or require considerable additional manual work and empirical adjustments for these types of applications.

In an effort to handle these problems, growing attention has been given to methods obtained by a variational approach when the interpolation function minimizes an appropriate functional which represents some measure of smoothness of this function. Probably the best known method obtained within this approach is minimum curvature (MINQ) interpolation with numerical finite-difference solution of the variational condition (Briggs, 1974). The main drawback of this method is the generation of overshoots, which appear in regions with rapid change of gradient; in addition, the numerical solution can be computationally costly. The method has been improved significantly by Hutchinson (1989) by adding first derivative terms to the variational condition that minimizes the overshoots and by incorporating a drainage enforcement algorithm for interpolation of digital elevation models. This method also uses a multi-grid approach to reduce the computational cost of the numerical solution.

Numerical solution of the variational condition is not needed when an explicit solution is known, as is the case with the thin plate spline (TPS) (Duchon, 1976; Dubrule, 1984); however, this function has not been used widely in geosciences because of its global character and consequent difficulties in application to large datasets. An approach to overcome this problem was suggested by Franke (1982b), who has proposed segmented processing with smooth overlaps. Hardy's multiquadric functions (Hardy 1971; Hardy, 1990) belong to the same class of methods and a connection of TPS to kriging has been proved (e.g., Wahba, 1990).

In this paper, further development of this approach is presented which widens the range of its application to bivariate and trivariate interpolation with direct estimation of first and second order derivatives (necessary, for example, for topographic analysis). The possibility of creating a surface with anisotropic tension also has been included. To make this approach useful for a wide range of practical applications in geosciences a segmentation procedure with flexible overlapping neighborhood for large datasets with heterogeneous data distribution has been developed.

In the following section, the basic principles of the variational approach are presented together with the new interpolation functions. Then, their properties are used in interpolation with a simple type of anisotropy and an algorithm for segmented processing is described. In the third section, test examples are given. Derivation of the interpolation functions together with the first and second order derivatives for the bivariate case are presented in the Appendix.

VARIATIONAL APPROACH TO INTERPOLATION

Several interpolation methods are based on the assumption that the interpolation function should be smooth. For example, Talmi and Gilat (1977) proposed to measure the smoothness of a given function $g(\mathbf{x})$, $\mathbf{x} = (x_1, x_2, \ldots,$

x_d), of d real variables in a considered region Ω of d-dimensional space via the following smooth seminorm $E(g)$

$$E^2(g) = \sum_\alpha B_\alpha \int \cdots \int_\Omega \left[\frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \ldots \partial x_d^{\alpha_d}} g(\mathbf{x}) \right]^2 dx_1\, dx_2 \ldots dx_d \quad (1)$$

where $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d)$ is a multi-index with nonnegative integer components, with

$$|\alpha| = \sum_i \alpha_i \quad (2)$$

and $\{B_\alpha\}$ are some nonnegative constants. Using the smooth seminorm (Eq. 1), the variational solution of the interpolation problem is formulated as follows:

Given N values of the studied phenomenon $z^{[j]}$, $j = 1, \ldots, N$ measured at discrete points $\mathbf{x}^{[j]} = (x_1^{[j]}, x_2^{[j]}, \ldots, x_d^{[j]})$, $j = 1, \ldots, N$ within a certain region of a d-dimensional space, find a function $z(\mathbf{x})$ which fulfills the conditions

$$z(\mathbf{x}^{[j]}) = z^{[j]}, \qquad j = 1, \ldots, N \quad (3)$$

$$E^2(z) = \text{minimum} \quad (4)$$

Under fairly general conditions, the problem has a unique solution (Talmi and Gilat, 1977), which can be expressed as the sum of two components

$$z(\mathbf{x}) = T(\mathbf{x}) + \sum_{j=1}^{N} \lambda_j R(\mathbf{x}, \mathbf{x}^{[j]}) \quad (5)$$

The "trend" function $T(\mathbf{x})$ is given by

$$T(\mathbf{x}) = \sum_{l=1}^{M} a_l f_l(\mathbf{x}) \quad (6)$$

where $\{f_l(\mathbf{x})\}$ is a set of linearly independent functions (monomials) which have zero smooth seminorm (Eq. 1). $R(\mathbf{x}, \mathbf{x}^{[j]})$ is a radial basis function with an explicit form which depends on the choice of $\{B_\alpha\}$ in the smooth seminorm (Eq. 1). Once the basis function is known, coefficients $\{a_l\}$, $\{\lambda_j\}$ are obtained by solving the following system of linear equations

$$z(\mathbf{x}^{[j]}) = z^{[j]}, \qquad j = 1, \ldots, N \quad (7)$$

$$\sum_{j=1}^{N} \lambda_j f_l(\mathbf{x}^{[j]}) = 0, \qquad l = 1, \ldots, M \quad (8)$$

With the proper choice of $\{B_\alpha\}$ in the smooth seminorm, various interpolation functions with desired properties can be derived. The mathematical background for construction of radial basis functions has been published by Talmi and Gilat (1977), and some new results for the two- and three-dimensional cases were derived in Mitáš and Mitášová (1988).

Interpolation Functions

The best known explicit interpolation function for $d = 2$ obtained within this approach is the thin plate spline (Duchon, 1976; Dubrule, 1984), which minimizes the smooth seminorm with second order derivatives only. The resulting interpolation function is a close approximation to the surface which minimizes the blending energy of a thin steel plate that is forced to pass through constraints representing the data points. Experience with TPS indicates that it gives good results for various applications (Mitáš and Novák, 1985; Mitášová, 1987); however, as for the MINQ method, problems arise if the modeled phenomenon has regions with rapid change of gradients. In this case, overshoots appear due to the plate's stiffness. The stiffness of the plate can be suppressed by including first derivatives to the smooth seminorm that leads to TPS with tension (Franke, 1985; Mitáš and Mitášová, 1988), which enables the character of the interpolation surface to be tuned from thin plate to membrane. However, for various applications, especially where analysis of the surface is required, these functions are not sufficiently general. They exhibit logarithmic divergencies of second derivatives at the data points, and consequently, direct estimation of curvatures becomes problematic. To remove this drawback, plate stiffness around data points have been increased by including third order derivatives to the smooth seminorm (Mitáš and Mitášová, 1988). Tests by Hofierka and Šúri (1989) indicate that the resulting function, regularized TPS with tension, is more accurate than other standard methods. However, the equations for the basis function and for the derivatives are involved and thus require more computational time.

Recently, we have derived new interpolation functions which will here be called completely regularized splines (CRS) (Appendix). The smooth seminorm of these functions includes derivatives of *all* orders in a manner similar to the one originally proposed by Talmi and Gilat (1977). Inclusion of derivatives of all orders with the proper weights enables relatively simple explicit expressions to be found for the basis functions for $d = 2, 3$. The resulting interpolation functions (Eq. 5) are as follows:

$$T(\mathbf{x}) = a_1, \qquad d = 2, 3 \tag{9}$$

so that the "trend" function is a constant ($M = 1$); the basis functions are given by

$$R(r_j) = -\left\{\ln\left[\left(\frac{\varphi r_j}{2}\right)^2\right] + E_1\left[\left(\frac{\varphi r_j}{2}\right)^2\right] + C_E\right\}, \qquad d = 2 \tag{10}$$

$$R(r_j) = \frac{1}{\varphi r_j}\,\mathrm{erf}\left(\frac{\varphi r_j}{2}\right) - \frac{1}{\sqrt{\pi}}, \qquad d = 3 \tag{11}$$

Here $r_j^2 = \Sigma_{i=1}^d (x_i - x_i^{[j]})^2$ and erf $(\cdot)$ and $E_1(\cdot)$ denote error and exponential integral functions, respectively. C_E (Eq. 10) is the Euler constant ($C_E = 0.577215 \ldots$). Functions (Eqs. 10 and 11) have regular derivatives of all orders everywhere and φ in this case can be considered as a generalized tension parameter. It tunes the ratio between weights of the first and higher order derivatives in the smooth seminorm (Appendix) and thus controls behavior of the resulting surface from membrane to a thin plate. The value of the generalized tension parameter has to be determined empirically. However, experience suggests that suitable values may be found within a few trials.

Tension Anisotropy

The presented interpolation functions have the following properties:

(i) They are invariant to a rotation of coordinate space because the basis functions depend only on distance.

(ii) They are *not* scale invariant, and change of scale is equivalent to change in the tension parameter φ (Eqs. 10 and 11).

The first property means that the character of the interpolant is direction independent. However, in many real situations, the modeled phenomena exhibit various degrees of anisotropy and the interpolation function should mimic this effect to a certain extent. For this purpose, the second property can be used, by rescaling one axis, the tension becomes different in this direction when compared with the original unscaled case. By rotation of coordinate space, the tension maximum (or minimum) can be oriented in any prescribed direction. For $d = 2$, the transformation from original coordinates $\mathbf{x} = (x_1, x_2)$ to new coordinates $\mathbf{x}' = (x'_1, x'_2)$ is simply

$$\mathbf{x}'^T = \mathbf{S}\mathbf{B}(\theta)\mathbf{x}^T \tag{12}$$

where T denotes transposition and $\mathbf{B}(\theta)$ is an orthogonal matrix that rotates the coordinate system around the origin by angle θ

$$\mathbf{B}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{13}$$

and $\mathbf{S}$ is a diagonal scaling matrix

$$\mathbf{S} = \begin{pmatrix} s_1 & 0 \\ 0 & s_2 \end{pmatrix} \tag{14}$$

where s_1, s_2 are scaling coefficients (one of which is usually equal to one). The generalization of the coordinate transformation for $d = 3$ is straightforward.

Segmentation for Large Datasets Processing

The quality of global interpolation methods (as TPS) has been recognized in several papers (e.g., McCullagh, 1988; Hutchinson, 1989); however, they were considered to have limited practical use. The reason is that the computational demands are proportional to N^3 (N is number of data points). This scaling comes from the solution of system of linear equations (Eqs. 7 and 8), and the method is prohibitively slow and possibly unstable when applied to large datasets. To overcome this limitation, an algorithm for segmented processing inspired by the approach proposed by Franke (1982b) was developed.

The idea of segmented processing is based on the fact that, for large datasets, the behavior of the interpolation function is local: this means that the interpolation function in some limited area is not sensitive to data at some, *sufficiently distant*, point. This is, in fact, a consequence of the condition given by Eq. (8), however, detailed analysis of this property is beyond the scope of this paper.

Using local behavior of the interpolation function, the following segmentation procedure was designed. The interpolated area is divided into a regular mesh of square segments (boxes). The optimal size of these segments is found by subsequent division of the area into finer and finer mesh until the number of data points in each segment plus its 3×3 neighboring segments is less than some specified maximum K_{max} (e.g., the number of linear equations that can be solved efficiently on a given computer).

To ensure the smooth connection of segments, values of the interpolation function in a given segment are computed using the points from this segment *and* from the neighboring ones (Fig. 1). If the number of points in the given segment and its 3×3 neighborhood is less than specified minimum K_{min}, the number of neighboring segments from which the points are taken into account is increased to 5×5 or more, until the number of points used for the interpolation is greater than K_{min}.

With flexible segmentation computer time and memory requirements for this interpolation procedure are proportional to N. It also allows interpolation of surfaces from strongly nonhomogeneous data (e.g., clustered, profile, or digitized contour data) by a proper choice of K_{max} and K_{min}. Typical values in applications for digitized contours with a large proportion of areas with sparse data (flat terrain) were $K_{max} \approx 300$ and $K_{min} \approx 200$; for more homogeneously distributed data, a smaller value of K_{min} makes computation more efficient (for example, for homogeneously distributed digitized contour data or data from climatic stations, $K_{min} \approx 100$ may be used).

Generalization of this procedure to the three dimensional case is straightforward. The segmentation procedure is not restricted to CRS. It can be used for other global interpolation functions, such as Hardy's multiquadric or kriging.

EXAMPLES FOR APPLICATIONS

Test of Accuracy

The accuracy of CRS was compared with other methods using the bivariate function proposed by Franke (1982a). This function was chosen because it was used in tests of several interpolation methods (e.g., Franke, 1982a; Renka and

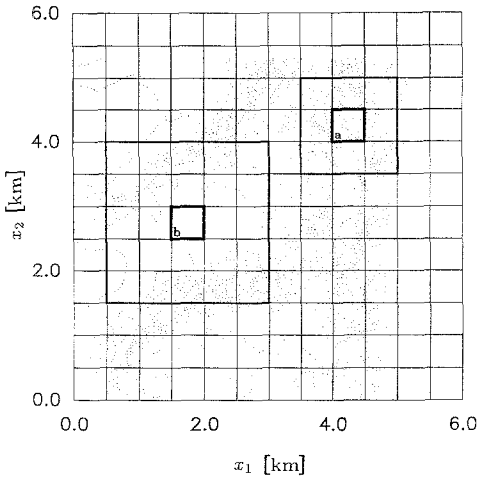

Fig. 1. Segmented processing. Interpolation function in the given segment (thick line) is computed from points in this segment and from points in the neighboring ones. For the segment **a**, 3 × 3 neighborhood is sufficient. For the segment **b** (flat area with sparse data), 5 × 5 neighborhood is used so that the number of points for interpolation is larger than the given K_{min} (see text).

Cline, 1984). The function is sampled by 100 scattered data points within the unit square (their coordinates were digitized from Fig. 5; Renka and Cline, 1984). The accuracy of the interpolation was tested at 33 × 33 regular grid points and compared with results obtained from other methods (Table 1). From these results, at least for this type of surface, CRS has the greatest accuracy.

Interpolation with Tension

The influence of tension on an interpolated surface is demonstrated on a bivariate function with fault, originally presented by Nielson and Franke (1984). The function was sampled over 33 scattered data points within the unit square (data were taken from Table 1; Nielson and Franke, 1984). The result of applying the thin plate spline to these data (Fig. 2) is similar to that obtained by several other standard methods (Nielson and Franke, 1984). The resulting surface exhibits a strong wavy behavior near the fault. By applying CRS with greater tension ($\varphi = 45$), overshoots were significantly minimized (Fig. 3). The effect of tension anisotropy is clearly visible (Figs. 4 and 5) where greater tension was applied in direction perpendicular and parallel to the fault, respec-

Table 1. The Mean and Maximum Absolute Errors of Various Bivariate Interpolation Methods for a Test Function[a]

Method	Mean error	Max. error
Akima Mod. III	0.00729	0.0520
Mod. quadr. Shepard	0.00785	0.0573
Lawson	0.00783	0.0951
Renka global	0.00540	0.0499
Renka local	0.00619	0.0505
Nielson–Franke quadr.	0.00741	0.0782
Nielson min. norm	0.00537	0.0492
Hardy quadric	0.00181	0.0225
Thin plate spline	0.00497	0.0470
Compl. reg. spline $\varphi = 10$	0.00290	0.0280
Compl. reg. spline $\varphi = 13$	0.00158	0.0168
Compl. reg. spline $\varphi = 20$	0.00323	0.0301

[a]The results for the first seven methods have been taken from Renka and Cline (1984), the result of Hardy's method from Hardy (1990).

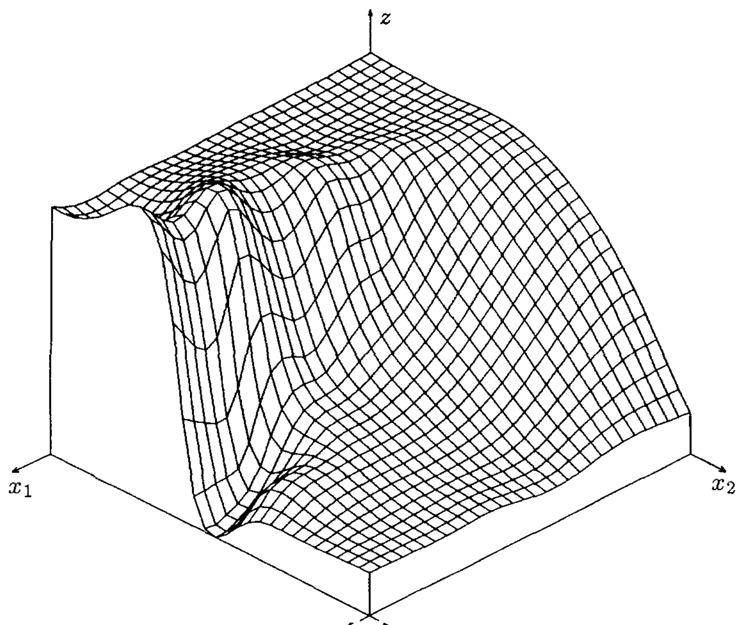

Fig. 2. Test function with fault interpolated from 33 scattered data points by thin plate spline.

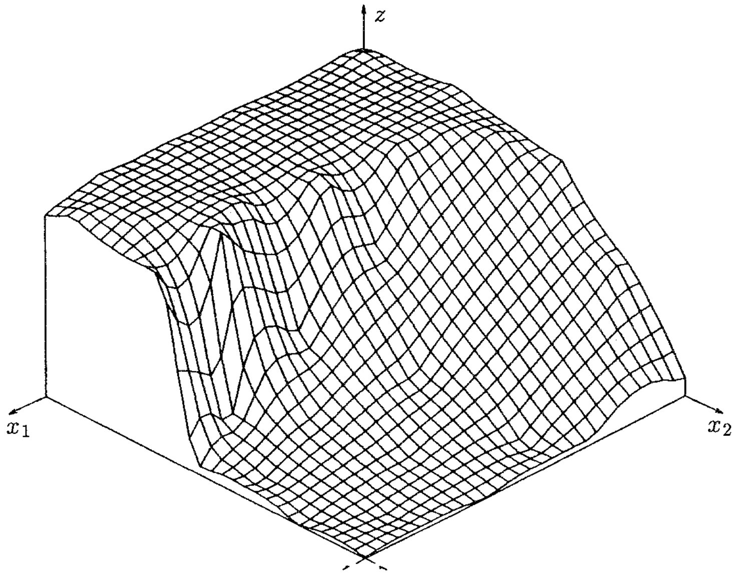

Fig. 3. Test function with fault interpolated by CRS with tension $\varphi = 45$.

tively. Note that all surfaces (Figs. 2–5) were obtained from the same data points, only tension was changed.

CONCLUSIONS

New interpolation functions are presented that integrate several important properties useful for the solution of a wide range of problems of surface modeling and surface analysis. The functions, bivariate and trivariate completely regularized splines, have the following properties:

(a) *Accuracy.* In comparison with other methods, on a simple test example, the bivariate function performed among the best, and with proper choice of the tension parameter it gave the most accurate results. For the trivariate case, accuracy was the same as or better than that of Hardy's method, depending on choice of parameters (Zlocha, 1990).

(b) *Flexibility.* The character of the resulting surface can be tuned from thin plate to membrane by the tension parameter. The tension parameter enables interpolation of surfaces with areas of rapid gradient change without excessive overshoots. Surfaces with a simple type of anisotropy can be modeled as well, using different tension in one direction. The generalized tension parameter has simple physical interpretation that makes the methods easier to use.

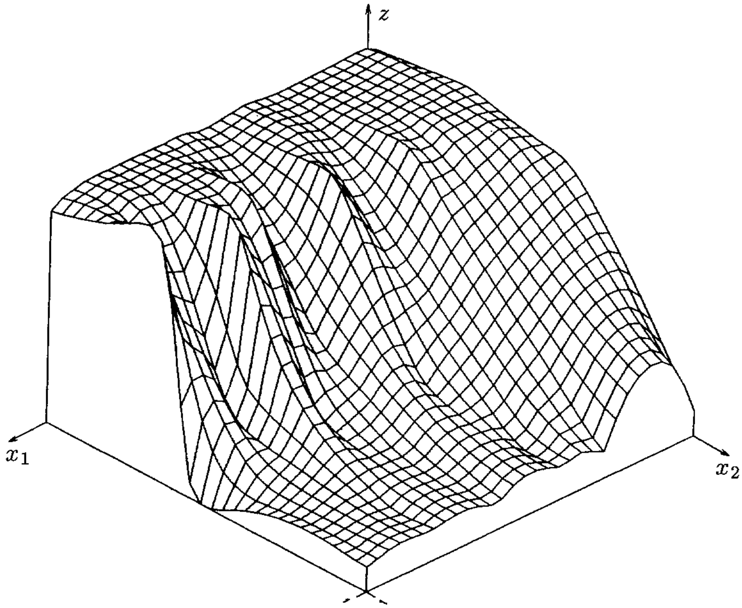

Fig. 4. Test function with fault interpolated by CRS with anisotropic tension (φ = 50, s_1 = 1, s_2 = 0.32).

(c) *Regular Derivatives of All Orders.* Derivatives of the interpolation function can be computed simultaneously with interpolation and directly used for surface geometry analysis.

(d) *Local Behavior (the Greater the Tension, the More Local the Behavior).* Local behavior enables application of segmented processing for large datasets (tens of thousands of data points). A procedure with automatic determination of optimal size of segment and flexible size of overlapping neighborhood has been developed for data with heterogeneous spatial distribution (digitized contours, clustered drill-hole data, etc.).

Presented method was incorporated into the public domain software for geographic information systems GRASS (Geographic Resources Analysis Support System) as command s.surf.tps (GRASS4.1 Reference Manual, 1993). It has been already successfully used for many applications, e.g., terrain modeling and analysis for the erosion risk assessment (Mitášová and Hofierka, 1993), interpolation of climatic data and climatic index of biomass productivity (Iverson et al., in press), volume modeling of geological deposit (Mitášová et al., 1990).

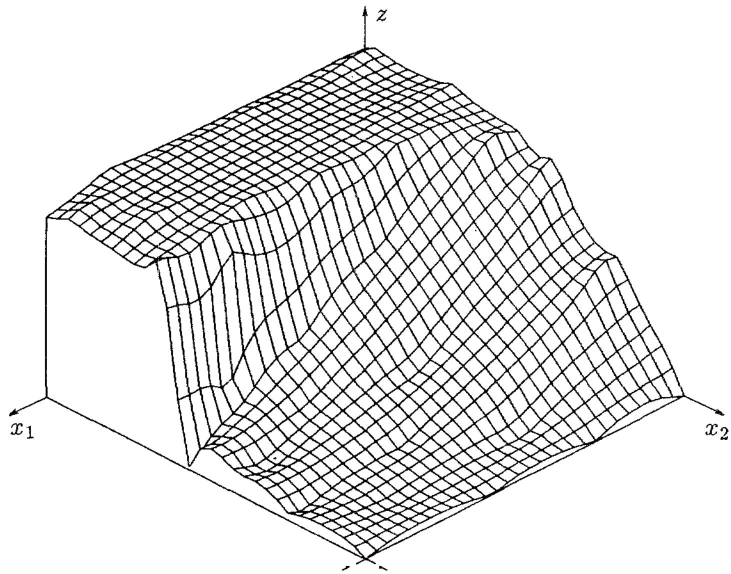

Fig. 5. Test function with fault interpolated by CRS with anisotropic tension (φ = 100, s_1 = 0.39, s_2 = 1).

The approach has significant potential for further development such as the addition of a cross-validation procedure for estimating the predictive error of interpolation and for smoothing of noisy data as described by Wahba (1990). Minimization of the predictive error obtained from cross-validation also could be used for automatic determination of the optimal tension parameter. Interpolation with prescribed derivatives can widen applications to problems with *a priori* information about gradients and singular points of the surface representing the modeled phenomenon (Talmi and Gilat, 1977).

APPENDIX

Completely Regularized Spline

Explicit expressions for the radial basis functions for bivariate and trivariate cases are derived according to formalism defined by Eqs. (1–8). Consider the smooth seminorm given by Eq. (1) with the following choice for coefficients

$$B_\alpha = \begin{cases} 0, & |\alpha| = 0 \\ \dfrac{C(\alpha)}{\varphi^{2|\alpha|}(|\alpha| - 1)!}, & |\alpha| > 0 \end{cases} \tag{A1}$$

where

$$C(\alpha) = \frac{|\alpha|!}{\alpha_1!\alpha_2! \ldots \alpha_d!} \tag{A2}$$

and φ is a relative reciprocal weight of particular terms in the sum (Eq. 1). Recall that $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d)$ and that each component can be any non-negative integer. With this particular choice of coefficients, the basis functions can be found explicitly while keeping the advantage of having regular derivatives of higher orders and the possibility of variable tension.

The "trend" function $T(\mathbf{x})$ is, according to Eqs. (1), (2), and (6), a constant

$$T(\mathbf{x}) = a_1 \qquad \text{for} \quad d = 2, 3 \tag{A3}$$

because only a constant has zero smooth seminorm with the coefficients given by Eq. (A1). Assuming that $\Omega = \Re^d$, where $\Re$ is the set of real numbers, the radial basis functions can be derived as follows. Previously, Talmi and Gilat (1977) and Mitáš and Mitášová (1988) have shown that the basis function can be expressed in the form of a Fourier integral

$$R(\mathbf{x}, \mathbf{x}^{[j]}) = \frac{1}{(2\pi)^d} \int_{\Re^d} \frac{\exp\,[i\mathbf{q} \cdot (\mathbf{x} - \mathbf{x}^{[j]})] - 1}{\sigma(\mathbf{q})}\, dq_1\, dq_2 \ldots dq_d \tag{A4}$$

where

$$\sigma(\mathbf{q}) = \sum_\alpha B_\alpha q_1^{2\alpha_1} q_2^{2\alpha_2} \ldots q_d^{2\alpha_d} \tag{A5}$$

and $\mathbf{q} = (q_1, q_2, \ldots, q_d)$.

Using Eqs. (A1) and (A2), the sum given by (A5) is simply

$$\sigma(\mathbf{q}) = \left(\frac{q}{\varphi}\right)^2 \exp\left[\left(\frac{q}{\varphi}\right)^2\right] \tag{A6}$$

where q is Euclidean length of vector $\mathbf{q}$. Equation (A6) can be substituted immediately in Eq. (A4). For the two-dimensional case, the double integral Eq. (A4) can be rewritten into a single one using the transformation to polar coordinates and integrating over the angular variable. The function under the integral then includes the ordinary Bessel function $J_0(\cdot)$, which is rewritten into power series. After the integration, term by term, and subsequent resummation

$$R(\mathbf{x}, \mathbf{x}^{[j]}) = R(r_j) = -\frac{\varphi^2}{4\pi}\left\{\ln\left[\left(\frac{\varphi r_j}{2}\right)^2\right] + E_1\left[\left(\frac{\varphi r_j}{2}\right)^2\right] + C_E\right\}, \quad d = 2 \tag{A7}$$

where E_1 is the exponential integral function (Abramowitz and Stegun, 1964) and C_E is the Euler constant ($C_E = 0.577215\ldots$). The multiplicative constant $\varphi^2/4\pi$ can be omitted because it can always be absorbed into coefficients $\{\lambda_j\}$ in Eq. (5) so that the basis function is given by Eq. (10).

The trivariate case is even more simple. After transformation to spherical variables and integration over angular variables, the remaining integral is tabulated (Gradshteyn and Ryzhik, 1980) and the basis function is given by

$$R(\mathbf{x}, \mathbf{x}^{[j]}) = R(r_j) = \frac{\varphi^3}{4\pi}\left[\frac{1}{\varphi r_j}\operatorname{erf}\left(\frac{\varphi r_j}{2}\right) - \frac{1}{\sqrt{\pi}}\right], \quad d = 3 \tag{A8}$$

where $\operatorname{erf}(\cdot)$ is the error function. The multiplicative constant $\varphi^3/4\pi$ can again be omitted and the basis function is given by Eq. (11).

Functions (A7 and A8) have regular derivatives of all orders everywhere and φ, in this case, is considered as a generalized tension parameter.

Finally, note that for the special functions $\operatorname{erf}(\cdot)$ and $E_1(\cdot)$, appropriate polynomial-like approximations can be found (Abramowitz and Stegun, 1964). However, radial functions and their derivatives should be evaluated carefully at small values of distance r_j because the function, say Eq. (A7) is then expressed formally as the difference of two large contributions which leads to an obvious numerical instability. This problem is solved by using a series expansion around the origin of the considered function (Abramowitz and Stegun, 1964). Then, the singular terms can be cancelled explicitly and evaluation of the remaining regular terms is without complication.

Derivatives for Bivariate Case

For the convenience of the reader, derivatives up to the second order of the basis function given by Eq. (10) are listed for the two-dimensional case. First, several definitions are introduced

$$\eta = \frac{\varphi}{2} \tag{A9}$$

$$R'(r_j) = 2\,\frac{1 - e^{-(\eta r_j)^2}}{r_j} \tag{A10}$$

$$R''(r_j) = 2\,\frac{[2(\eta r_j)^2 + 1]e^{-(\eta r_j)^2} - 1}{r_j^2} \tag{A11}$$

Partial derivatives can be expressed as follows

$$\frac{\partial R(r_j)}{\partial x_l} = R'(r_j) \frac{(x_l - x_l^{[j]})}{r_j}, \qquad l = 1, 2 \tag{A12}$$

$$\frac{\partial^2 R(r_j)}{\partial x_1^2} = R''(r_j) \frac{(x_l - x_1^{[j]})^2}{r_j^2} + R'(r_j) \frac{(x_2 - x_2^{[j]})^2}{r_j^3} \tag{A13}$$

whereas the second derivative, according to x_2, is found easily from Eq. (A13) by exchange of indexes 1 and 2. The mixed derivative is given by

$$\frac{\partial^2 R(r_j)}{\partial x_1 \partial x_2} = \left[R''(r_j) - \frac{R'(r_j)}{r_j} \right] \frac{(x_1 - x_1^{[j]})(x_2 - x_2^{[j]})}{r_j^2} \tag{A14}$$

Numerical Stability and Parameter φ

Stability of the system of linear Eqs. (7) and (8) is dependent on the tension parameter φ. For a given number of equations (say, about 300), an interval (φ_0, ∞) of values for the parameter φ exists when the solution is stable. The instability can be detected after solving of the system of Eqs. (7) and (8) by a test whether the interpolation function reproduces the original data, that is, whether the interpolation condition (Eq. 3) is fulfilled (within some prescribed tolerance). If $\varphi < \varphi_0$, the difference between the original and interpolated value is intolerably large and the instable régime of φ parameter prevails. Fortunately, this instability is not important from a practical point of view. The important point is that small values of tension φ (say, $\varphi \approx \varphi_0$) give surfaces with artificial structure with many overshoots. This is a consequence of the fact that small values of φ give large weight to high derivative members in the seminorm (Eq. 1). However, for most practical tasks, only first, second, and third derivatives are really important so the "optimal" value of φ is always larger than φ_0.

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