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RECENT ADVANCES IN THE APPROXIMATION OF SURFACES FROM SCATTERED DATA

by

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Advances in the mathematical theory behind Hardy's multiquadric method, development of methods for surfaces with tension parameters or which satisfy constraints, and methods for least squares approximation and subset selection are discussed. This report was prepared for the proceedings of The International Workshop on Multivariate Approximation, held in Santiago, Chile, in December 1986.

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1.0 Introduction

The problem of interpolating or approximating data from scattered measurements arises in many areas of science and engineering. The importance of the problem has resulted in a large number of methods for solution of the problem, as has been noted in surveys by Schumaker [55], Barnhill [4], and more recently by Franke [19]. The problem can be described very easily. Given data (x_i,y_i,f_i), $i=1,\ldots,N$, construct a (smooth) function, $F(x,y)$ such that $F(x_i,y_i) = f_i$, $i=1,\ldots,N$. No assumption is made regarding the spacing of the independent variable data. More generally, especially when the data are subject to errors, one may wish to relax the interpolation condition and approximate the surface. The problem has an obvious generalization to more independent variables. The existence of many methods for such a surface is due to the many sources of data and the great number of possible dispositions of data points. Some advice on how to proceed for given data is contained in Sabin [50]. It is clear that no one method is satisfactory for all cases.

In the last few years a number of advances have been made. Because of space and time limitations, this paper will be confined to a few of those which I feel to be particularly important or interesting. The first area concerns the mathematical underpinnings of the multiquadric method of Hardy [22]. This method has previously been noted to work well in a variety of cases (see Franke [19] and Kansa [29], for example), but until recently little was known in terms of a mathematical theory for the method. These developments will be reviewed in section 2. The

construction of surfaces with tension parameters or satisfying constraints seems to be desirable based on the importance of such ideas in the univariate case, and recent results are discussed in section 3. Finally, since the amount of data is sometimes far in excess of what is required to define a sufficiently accurate surface, the problem of surface approximation and selection of subsets on which to base interpolating (or approximating) surfaces has become important, and this topic will be treated in section 4.

There have been other developments which are important, but will not be treated here. These include convergence of Shepard's method (see Farwig [17]), interpolation on the sphere (see Lawson [32], Wahba [63], Renka [49], Ramaraj [48], and Nielson and Ramaraj [46]), and some new implementations of "finite element" methods and related things such as derivative estimation and new, higher order elements (see Alfeld [2-3], LeMehaute [33], [34], Sablonniere [51]). Certain methods based on statistical ideas (especially Kriging in geology and Optimum Interpolation in meteorology) continue to be the focus of much effort in those particular disciplines. Relevant recent references include Journel [28] and Thiebaux [59].

2.0 Multiquadrics and Related Methods

The multiquadric (MQ) method was proposed by Hardy [22], and he has investigated the fitting properties of the method when applied to data from various sources in a series of papers that have appeared since that time [23-25]. The scheme is quite simple to implement and is reasonably efficient in terms of

computer resources provided the number of points is not large. A basis function (a quadric) $B_j = (d_j^2 + r^2)^{1/2}$ is associated with the j^{th} data point. Here d_j is the distance from the point (x,y) to the j^{th} data point (x_j,y_j) and r is a parameter in the method. Note that each of the basis functions is a radial function with respect to the data point, and that they are all translates of each other, which overcomes the usual problem of running afoul of the Haar theorem regarding interpolation in more than one variable. Now, a linear combination of the functions

$$F(x,y) = \sum_{j=1}^{N} a_j B_j(x,y)$$

is required to interpolate the given data. This yields the system of equations,

$$\sum_{j=1}^{N} B_j(x_i,y_i)a_j = f_i \quad , \quad i=1,2,\ldots,N$$

The existence of the interpolant is dependent on the nonsingularity of the matrix $\{B_j(x_i,y_i)\}$. Other authors have also investigated the scheme, generally from an empirical point of view [19], [27], [57]. These authors have found that the method is quite adept at yielding good approximations, in many situations better than any other method. In addition to this method, the use of the reciprocal of the above basis function leads to the "reciprocal" MQ method.

The MQ method is one of a class that I have previously called "global basis function methods", and which others have called "kernel" methods. In general the approximation takes the form

$$F(x,y) = \sum_{j=1}^{N} a_j B_j(x,y) + \sum_{j=1}^{M} b_j p_j(x,y) ,$$

where $\{p_j\}$ is a set of monomials of degree <m. The equations for the coefficients in such methods may be written in the form

$$\sum_{j=1}^{N} B_j(x_i,y_i)a_j + \sum_{j=1}^{M} p_j(x_i,y_i)b_j = f_i, \quad i=1, \ldots,N \quad .$$

$$\sum_{j=1}^{N} p_i(x_j,y_j)a_j \quad = 0 \quad , \quad i=1, \ldots ,M \quad .$$

The first of the equations require interpolation to the data by a linear combination of the basis functions $B_j(x,y)$ plus the M polynomial terms, $p_j(x,y)$, while the last set requires the coefficients to satisfy a certain constraint, which as we shall see, may related to the conditional positive definiteness of $\{B_j(x_i,y_i)\}$, and serves to guarantee exactness for the set of polynomials $\{p_j(x,y)\}$. In matrix form, we may write

$$\begin{pmatrix} A & E \\ E' & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} f \\ 0 \end{pmatrix} .$$

2.1 The Multiquadric Method: Theory

The intriguing aspect of the method is that until recently, very little was known in terms of a mathematical basis for the efficacy of the method, even whether or not the coefficient matrix was possibly singular. As recently as 1983 at The International Symposium on Surface Approximation, in Gargnano, Italy, I proposed as a conjecture the inequality

$$(-1)^{N-1} \det\{B_j(x_i,y_i)\} > 0 .$$

As it turned out, Charles Micchelli promptly heard of the conjecture, and subsequently proved it, and along the way, theorems

which answered some other questions as well.

To discuss the results of Micchelli [41] it is necessary to define some terms and give some background information. Because of the generalization to s-dimensional space, for this discussion, points in R^s will be denoted as (possibly superscripted) boldface vectors rather than subscripted coordinates.

Definition: A continuous function F(t), defined on $[0,\infty)$ is said to be conditionally (strictly) positive definite of order k on R^s if for any distinct points $\mathbf{x}^1$, $\mathbf{x}^2$, ..., $\mathbf{x}^n$ in R^s, and scalars c_1, c_2, ..., c_n such that

$$\sum_{i=1}^{n} c_i p(\mathbf{x}^i) = 0$$

for all polynomials p over R^s of degree $<k$, the quadratic form

$$\sum_{i=1}^{n}\sum_{j=1}^{n} c_i c_j F(||\mathbf{x}^i - \mathbf{x}^j||^2)$$

is (positive) nonnegative.

Let the class of functions which are conditionally positive definite of order k over R^s be denoted by $\mathbf{P}_k(R^s)$, and the class of functions which are conditionally positive definite of order k over R^s, for all s, by $\mathbf{P}_k$. Further, recall that a function F is completely monotonic on $(0,\infty)$ if it is in $C(0,\infty)$ and $(-1)^m F^{(m)}(t) \geq 0$ for all $t>0$ and $m=0,1,2,\ldots$.

Theorem 1: F is in $\mathbf{P}_k$ whenever F is continuous on $[0,\infty)$ and $(-1)^k F^{(k)}(t)$ is completely monotonic on $(0,\infty)$.

This theorem is due to Schoenberg [54] for order k=0. Further, if F is not a polynomial of degree $\leq k$, and if the points in

the definition of completely monotonic are distinct, then the quadratic form is positive. Take $F(t) = (r^2+t)^{1/2}$, and note that for $m \geq 1$, $F^{(m)}(t) = C_m(-1)^{m-1}(r^2+t)^{(1-2m)/2}$, where C_m is a positive constant. This special case leads to the coefficient matrix for the MQ method, which is seen to be conditionally positive definite of order k=1.

When the constant r is taken to be zero, each basis function is the upper half of a cone, hence the interpolant is not smooth at the data points. This particular interpolant is almost the "multiconic" method of Duchon [13]. The difference is that the multiconic approximation is consistent with the concept of conditional positive definiteness of order one. The overall approximation takes the form of a linear combination of the basis functions plus a constant, with the additional constraint that the coefficients satisfy,

$$\sum_{j=1}^{n} a_j = 0 \quad .$$

This constraint is easily seen to guarantee precision for constant functions. This special case, along with Theorem 1, is convincing evidence that a constant and the corresponding constraint should be included in the MQ approximation. In a practical vein, however, my own limited tests have indicated that the accuracy of the method is not always helped, and may be hindered, by including the constant.

The "reciprocal" MQ method uses $2F'(t)$ for the basis function, and thus the theorem shows that the coefficient matrix for that scheme is positive definite.

Theorem 2: Let $l=[s/2]-k+2$ be a positive integer. Then for any function defined on $(0,\infty)$ such that $(-1)^{k+j}F^{(k+j)}(t)$ is nonnegative, nonincreasing, and convex for $j=0, 1, \ldots, l-2$ on $(0,\infty)$ (if $l=1$, we require only that it be nonnegative and nonincreasing), it follows that $F(\sqrt{t})$ is in $\mathbf{P}_k(R^s)$.

Theorem 3: Suppose F' is completely monotonic but not constant on $(0,\infty)$, F is continuous on $[0,\infty)$ and positive on $(0,\infty)$. Then for any distinct vectors $\mathbf{x}^1, \mathbf{x}^2, \ldots, \mathbf{x}^n$ in R^s (s arbitrary)

$$(-1)^{n-1}\det\{F(||\mathbf{x}^i-\mathbf{x}^j||^2)\} > 0 .$$

This last theorem proves the conjecture about the coefficient matrix in the MQ method. However, the theorem also yields similar results for interpolation by other sets of radial basis functions. Some of those methods are known by other results to always lead to nonsingular systems of equations, such as the "thin plate splines" of Duchon [12-13] (see also Harder and Desmarais [21] and Meinguet [37-40]), which are known to be nonsingular because of their semi-Hilbert space setting. Others, such as the basis function $\log(1+||\mathbf{x}-\mathbf{x}^j||^2)$ suggested by Dyn [16] are also seen to be positive definite of order $k=1$.

Another result of interest in specific applications has been obtained by Hardy and Nelson [26]. This result shows that the MQ method has a basis for approximation of geodetic and gravitational anomalies. The connection comes through the representation of the disturbing potential at point i due to anomalous disturbances as a three dimensional integral,

$$T_i = \int_V d_i \; p \; dV \; ,$$

where d_i is the distance from the point i, p is the Laplacian of the disturbing potential, and V is the volume of interest. What Hardy and Nelson showed is that the MQ method can be interpreted as a quadrature approximation to the above integral, one that is required to yield the correct result at certain (the data) points. While this particular result may say little about the scheme as a general interpolation scheme, it is interesting that such an interpretation exists for one of the early the uses of the method.

The role of the parameter r in the MQ method has long puzzled investigators. The original interpretation given by Hardy was a three dimensional one: His applications were actually in 3-space, and this value simply represented the z coordinate of the locations of the disturbing (point) potential. Given that the method performs so well, it seems likely that the MQ approximation can be described as approximation in some Sobolev-like space similar to that for the multiconic method. A recent development by Madych and Nelson [35] gives this result. The MQ method does minimize a certain pseudonorm involving a weighted integral. Further, the result applies to other similar schemes, and thus may also lead to ways of deriving other approximations with desired properties through explicit minimization of weighted pseudonorms. If practical for computational purposes, such results could have far reaching implications in applied scattered data approximation.

2.2 Multiquadric Method: Practice

In addition to the developments on the mathematical aspects

of the MQ method, some progress has been made in attempting to solve such systems of equations by iterative means. A series of investigations by Dyn and coworkers [15-16] have studied the problems of fitting scattered data with linear combinations of radial basis functions. The basic idea comes from the fact that thin plate splines have basis functions which are the fundamental solution of the biharmonic equation. The MQ basis functions are solutions of Laplace's equation (in three dimensions). Thus, when certain finite difference approximations to the iterated Laplacian are applied to the equations, the resulting equations tend to have a large diagonal term, which then yields a system of equations amenable to solution by iterative schemes. This process may be thought of as applying a conditioning operator to the system of equations.

The idea of the conditioning operator is to transform that part of the system of equations involving A into an equivalent one which is better conditioned, perhaps even diagonally dominant. In addition to transforming A suitably, the operator is constructed to annihilate E. This yields a singular system $CAa = Cf$, which has a unique solution, subject to the constraint $E'a = 0$.

Construction of the conditioning operator involves triangulation of the convex hull of the data point locations. Finite difference operators are then derived which approximate the necessary derivatives on the basis of the function behavior at the vertices of the triangles. Some care is necessary to ensure that the operators annihilate E, which corresponds to annihilating all polynomials of degree $<m$ on the given set of data points.

The results of applying these ideas to only a limited number of irregular, but "quasi-regular" grids are reported in [16]. Nonetheless, the results are very encouraging, with the condition number of the matrix being decreased by factors of up to 200 or more for the MQ method with up to 121 data points. In addition to the MQ method, the ideas are applicable to approximation by thin plate splines and other radial functions, and these are reported on as well.

One further interesting aspect of iterative schemes based on this conditioning is that for the MQ method, shifted logarithm ($\log(d^2 + r^2)$) basis functions, and shifted thin plate spline ($(d^2 + r^2)\log(d^2 + r^2)$) basis functions certain nice spectral properties of the matrix CA seem to occur. In particular, it was noted that computationally, the "rough" eigenvectors correspond to the smaller eigenvalues. Certain iterative schemes will remove those components quickly, leaving the surface corresponding to the approximate solution (before iteration to convergence) as a smooth one. Thus, terminating the iterative scheme prematurely corresponds to a smoothing scheme. Numerical evidence and examples are given by Dyn, Levin, and Rippa [16]. See [14] in this Proceedings for more recent results.

3.0 Surfaces with Tension or Constraints

In the univariate case, development of curves with tension parameters, constrained approximation, and monotone and convex approximation is at a high level. In each situation, several reasonable schemes for obtaining such approximations are readily available. In two or more independent variables, for scattered

data, the situation is not nearly so well developed. Indeed, the idea of exactly what characterizes monotone behavior of scattered data has not yet been clearly given. Nonetheless, there have been some noteworthy developments in the general area of surfaces with tension and surfaces satisfying certain constraint relationships, both from theoretical and computational points of view.

3.1 Tension

A generalization of splines under tension to the scattered data case was given by Nielson and Franke [45]. The basic idea is that of approximation of the the surface by a "finite element" method, such as proposed by numerous authors, among them Dooley [10], Akima [1], Lawson [31], Nielson [43], and LeMehaute [33]. The first step of this process consists of triangulation of the x-y data in some reasonable way (e.g., using the max-min angle criterion). A certain "finite element" function is assumed over each triangle. Ordinarily one wants a smooth surface, so at least C^1 functions are usually used. Depending on the element chosen, certain derivatives must be estimated from the data. It is this stage of the process which is crucial to the effectiveness of the method (see Nielson and Franke [44]).

The incorporation of tension into the approximation is achieved in the following manner. Let the vertices (x-y data pairs) of the triangulation be denoted by the set $\{V_i\}$, an index set of triangle edges joining V_i and V_j by N_e, and the edges of the triangulation by the set $\{e_{ij}: ij \epsilon N_e\}$. The ordering of the edges relative to the ordering of the data points is unimportant, but each edge must appear only once in the set. Let E be the

union of the set of edges. Define the set of functions C(E) as those which are C^1 over the convex hull of the $\{V_i\}$, restricted to E. Let the vector $\langle \alpha_{ij} \rangle$ be given, with nonnegative components, each corresponding to a tension parameter for the ij^{th} edge. Now define the pseudonorm

$$S_{\alpha}(F) = \sum_{ij \in N_e} \int_{e_{ij}} [(\frac{\partial^2 F}{\partial e^2})^2 + \alpha_{ij}^2 (\frac{\partial F}{\partial e})^2] \, de_{ij}$$

There is a unique minimizer of $S_{\alpha}(F)$ over all curve networks in C(E) which interpolate the data. That minimizer is the function which is a piecewise Hermite exponential (a linear combination of 1, u, $\exp(\alpha_{ij}u)$, $\exp(-\alpha_{ij}u)$, where u represents Euclidean distance along the edge, that takes on prescribed value and derivative conditions at the endpoints), and satisfying a certain system of (sparse) linear equations for the partial derivatives at the vertices. Asymptotic properties are as anticipated. For simplicity, take all tension parameters to have the same value, and then as tension goes to zero, the curve network approaches the curve network minimizing the corresponding functional, as developed previously by Nielson [43]. As the tension becomes large, the curve network approaches the piecewise linear network over the edges.

After obtaining the curve network over the edges of the triangulation, the surface is then completed using a C^1 blending method on the individual triangles. It is desirable to propogate the effects of tension into the interior of the triangles, so the previously known cubic blending techniques are inadequate. The method used was an extension of the side-vertex scheme (see

Nielson [42]) where the radial projectors were taken to be exponential Hermite functions. The net effect of the tension becoming large is that the surface tends toward the the surface which is piecewise linear over the triangulation.

The limiting behavior of the above construction is not the physical analog of the limiting behavior of a thin plate under tension. In an effort to model the behavior of the thin plate under tension in two independent variables, Franke [20] developed a surface which is the analog of the spline under tension in the same way that thin plate splines are the two dimensional analog of cubic splines. The "engineering" approach of Harder and Desmarais [21] is followed. The idea is to use superposition of fundamental solutions for a plate with tension to model the displacement under point loads. The fundamental solution (under appropriate assumptions about the plate parameters) satisfies

$$\Delta^2 W - \alpha^2 \Delta W = \delta \ ,$$

where α is a tension parameter. The solution is

$$W_\alpha(r) = (2\pi)^{-1} \int_0^r t^{-1} \int_0^t s K_0(\alpha s)\, ds dt + C \ ,$$

where, K_0 is the modified Bessel function. The solution to the interpolation problem is obtained by using this basis function (C is taken to be zero) in a global basis function method with m=1. Some experimentation was performed including linear polynomial terms, since this is more consistent with thin plate splines.

For tension $\alpha = 0$, the equation for the thin plate spline is attained, and as tension gets large, the equation becomes the membrane equation, which has no finite solution under point

loads. Examples are given which demonstrate that as tension is increased the surface tends to behave somewhat like a rubber sheet under point loads: too thick to be a membrane, but supporting little displacement away from the data points.

Construction of surfaces under tension has also been considered by Terzopoulous [58]. These surfaces are the analog of surfaces constructed by Briggs' method [6], although the paper also addresses the solution of the system of equations by multigrid methods. That appears to be quite effective, but will not be addressed here. In addition, as with Briggs' scheme, the best situation is when the data points all lie on a subset of a rectangular grid. The present development has only a C^0 underlying surface, which simplifies the calculations for minimization of the functional.

The idea is to minimize the sum of a penalty functional measuring closeness of fit to the data and the functional

$$\int_{D'} \rho(x,y)\{\tau(x,y)(F_{xx}^2+2F_{xy}^2+F_{yy}^2) + (1-\tau(x,y))(F_x^2+F_y^2)\}dA ,$$

where D is the region of interest in the plane, $\rho(x,y)$ is the "rigidity" of the plate and $0\leq\tau(x,y)\leq 1$ is the "surface tension". A rectangular grid is placed over the region D. While not necessary in practice, for simplicity it is assumed that the data points coincide with grid points. A nonconforming piecewise quadratic finite element is assumed, and the equivalent finite difference equations for the above functional are derived. These equations are solved by multi-grid techniques. Local tension can be achieved by allowing the tension parameter to vary over the grid points. Discontinuities in derivative and value are also

considered. As with Briggs' method, the final form of the approximation depends on the grid at which it is evaluated. Unlike Briggs' scheme, which is based on finite difference approximations to the plate equation, the underlying surface (although C^0) would allow evaluation at other than grid points.

3.2 Constraints

The construction of approximations satisfying inequality constraints as well as interpolation conditions has been investigated by Villalobos [62], and Dubrule and Kostov [11]. The former considered a generalization of Laplacian smoothing splines (see Section 4.1), while the latter considers only interpolating functions. The results are similar, and the latter will be described here. The discussion centers on approximation by thin plate splines. The functional minimized is the usual thin plate functional, but under the given constraints. As had been previously shown by others, the solution involves adding basis functions at constraint points that are found to be active, and is solved as a quadratic programming problem. This method appears to be easy and effective. The practical aspects of the method are discussed in the companion paper [30], where the process is applied using Kriging, which formally includes thin plate splines as a special case. Journel [28] discusses the incorporation of this and other "soft" information into the approximation by Kriging.

A more general problem and its elegant solution is considered by Utreras [61]. Here the problem is that of minimizing the thin plate functional,

$$\int_{\mathbb{R}^2} (F_{xx}^2+2F_{xy}^2+F_{yy}^2)\ dA$$

subject to interpolation conditions, and positivity conditions on a certain subset of the plane, say

$$F(x,y) \geq 0 \text{ for } (x,y) \in \mathbb{K} \subset \mathbb{R}^2.$$

Here the region $\mathbb{K}$ is assumed compact and convex. The existence and uniqueness of the solution is proven using elementary means. The characterization of the solution of the problem is in terms of the points where the constraints are active. Distribution theory and the relationship of the functional minimized to the biharmonic equation are used to show that the solution involves the usual terms of the thin plate spline approximation plus a certain term which serves to enforce the positivity of the function over the compact region $\mathbb{K}$.

We digress to introduce some notation. Suppose that scattered data is given with $f_i \geq 0$. Let $F(x,y)$ be the solution of the constrained problem which interpolates this data. Define the set $\mathbb{K}' = \{(x,y) \in \mathbb{K} : F(x,y) = 0\}$. $\mathbb{K}'$ is compact. Let $B_k(x,y) = d_k^2 \log d_k$, where $d_k^2 = (x-x_k)^2+(y-y_k)^2$, and $d_0^2 = x^2+y^2$. The following theorem, where * denotes convolution, is then proved.

Theorem: There exist constants a_i and a positive measure $\mathfrak{m}$ with support contained in $\mathbb{K}'$ such that

$$F(x,y) = \sum_{k=1}^{N} a_k B_k(x,y) + \mathfrak{m} * B_0(x,y) + p_1(x,y) ,$$

where p_1 is a polynomial of degree ≤ 1, and

$$\sum_{k=1}^{N} a_k q(x_k,y_k) + \mathfrak{m}(q) = 0$$

for any polynomial q of degree ≤ 1.

Convergence is investigated, and an algorithm is given for computing an approximation to the positive thin plate spline. The algorithm involves finding an approximation of the set K' and the measure μ such that the constraint is satisfied to within some tolerance. The approximation is by points with atomic measure, and since convolution with atomic measures give point evaluation, the solution is approximated by functions of the same type as in the Dubrule/Kostov program. The crucial difference is that here the constraint set K' must be completely discovered as part of the process, rather than being part of a finite subset specified in advance.

4.0 Smoothing, Least Squares, and Subset Selection

In many applications the data is obtained by measurement, often not to enough accuracy to warrant interpolation. In other applications, such as oceanography and remote sensing, the amount of data available, even though subject to errors, is much greater than is necessary to define the desired surface to the required accuracy. In these cases is is necessary to apply some smoothing process or to perform least squares approximation with some function having far fewer parameters than the number of data points. The theory of smoothing splines in several variables is well developed. For purposes of contrasting that idea with those of least squares and subset selection, a brief discussion of smoothing splines will be given.

4.1 Laplacian Smoothing Splines

Laplacian smoothing splines are a generalization of univariate smoothing splines to several variables along the same

direction as thin plate splines for interpolation. They were mentioned by Harder and Desmarais [21] in their seminal paper for the bivariate case under the physical interpretation of having forces applied at the data points through springs with various spring constants. This caused the surface to tend toward the data points, but the not necessarily to pass through them.

The mathematical development of Laplacian smoothing splines in the general case is given in Wahba and Wendelberger [64]. The notation of Section 2.1 for points in s-dimensional space will be followed in this discussion. The functional minimized in the case of smoothing splines is

$$N^{-1}\sum_{j=1}^{N}[F(\mathbf{x}^j)-f_j]^2/\sigma_j^2 \quad + \quad \lambda J_m(F) \quad ,$$

where J_m is the pseudonorm associated with interpolating splines, and λ is a smoothing parameter which governs the fidelity with which the surface fits the given data. Here it has been assumed that the errors are uncorrelated and have standard deviation σ_i at the point $\mathbf{x}^i$. The case of correlated errors is addressed briefly in Wendelberger's thesis [65].

Let $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_s)$ be a multi-index for partial differentiation (denoted by $F_{\boldsymbol{\alpha}}$), with each integer $\alpha_i \geq 0$ and $|\boldsymbol{\alpha}| = \alpha_1+\alpha_2+ \ldots +\alpha_s$. Then

$$J_m(F) = \sum_{|\boldsymbol{\alpha}|=m} \int_{R^s} (F_{\boldsymbol{\alpha}})^2 \, d\mathbf{x} \quad .$$

In this functional one can think of m as a smoothness parameter, the approximating functions being smoother (having higher order derivatives) the larger m is. In order for the required func-

tions to be in the appropriate spaces, it is necessary that $m>s/2$.

The solution of the problem is of the same form as thin plate splines,

$$F(\mathbf{x}) = \sum_{j=1}^{N} a_j B_j(\mathbf{x}) + q_{m-1}(\mathbf{x}) \quad ,$$

where the coefficients a_j and the coefficients $b_{\boldsymbol{\alpha}}$ of q_{m-1}, a polynomial of degree m-1, satisfy the system of equations

$$\sum_{j=1}^{N} a_j [B_j(\mathbf{x}^i) + N\lambda\sigma_j^2\delta_{ij}] + \sum_{|\boldsymbol{\alpha}|<m}{}' b_{\boldsymbol{\alpha}}(\mathbf{x}^i)^{\boldsymbol{\alpha}} = f_i \quad , \quad i=1,2, \ldots ,N$$

$$\sum_{i=1}^{N} a_i (\mathbf{x}^i)^{\boldsymbol{\alpha}} = 0, \qquad |\boldsymbol{\alpha}|<m.$$

In the above equations, δ_{ij} is the Kronecker delta, and $(\mathbf{x})^{\boldsymbol{\alpha}} = x_1^{\alpha_1} x_2^{\alpha_2} \ldots x_s^{\alpha_s}$.

The smoothing parameter λ must be specified before the smoothing spline can be computed, and Wahba and Wendelberger suggest the use of Generalized Cross Validation (GCV) to select the value. Although there is some evidence that GCV leads to undersmoothing (see Seaman and Hutchinson [56]), Utreras [60] has shown that GCV yields convergence under reasonable conditions. GCV can also be used to decide on the smoothness parameter, m, to be used, as well. A limitation of the scheme is that it is difficult to compute when there are more than 200-300 data points, since the problem involves the solution of a system of more than N linear equations, although techniques such as those of Dyn, described in the previous section, could be useful here.

4.2 Least Squares Approximation

Least squares approximation to scattered data is an approximation with (presumably many) fewer basis functions than there are data points. The problem at hand here, then, is to select the basis functions. Previous work has been done using tensor product cubic splines, and a number of authors (see [7], [8], [9], for example) have considered the problem. Several computer programs are available, and such methods are probably desirable for cases where data is somewhat uniformly distributed. In cases where the data is of greatly varying density, the use of tensor products results in knot locations on a grid, and this may not reflect the actual disposition of data points. In fact, there could be knots with no data nearby. While such problems are not insurmountable, they lead to nonuniqueness of the solution, and the minimum norm solution tends to not be aesthetically pleasing.

For varying density of data points it seems desirable to have flexibility in knot placement, and this leads to the idea of least squares approximation by thin plate splines. The MQ approximations also could be used, however the discussion will be in terms of thin plate splines, and the points at which these basis functions are centered will be referred to as "knot" points. Treatment of the knot point locations as parameters in the minimization process is possible, and has been reported upon by Schmidt [53]. The paper is brief, with few details of the algorithm being given. The initial knot configuration was taken to be of tensor product form, which may be apparent from the final configuration of knots in the examples given. The overall minimization process is a large nonlinear one, and if the

problems of one dimension carry over as one might expect, may be complicated in that knots may coalesce and the solution may not be unique. In addition it is likely true that the objective function may have many local minima, so an algorithm to search for a better local minimum, or to avoid a poor local minimum would be necessary.

The problem with treating the knot locations as parameters presently seems to be intractable mathematically, and for many knots is computationally expensive, with results obtained being of questionable quality. A different point of view on the problem is considered in McMahon [36], and a summary of his approach and results will be given.

The main problem in the process is the selection of knots, for once these have been decided upon, what remains is to solve the equations in the least squares sense, in principle an uninteresting task. If the selection of knot locations is to be decoupled from the least squares process, some assumption must be made order to have an algorithm for selection of the knots. The assumption in this case is that the independent variable data reflects something about the behavior of the dependent variable. For example, perhaps the density of data point locations is dependent on the curvature of the surface, or more broadly, if the function is changing behavior rapidly the density of data points is great, whereas low density indicates slowly changing behavior. This assumption is not universally satisfied in practice, for some data is taken based on accessibility (along roads in rugged areas, for example) or other nonbehavioral criteria.

The assumption of data density indicating local behavior of

the surface has a companion assumption that each data point is in some sense equally important in defining the function, regardless of whether it has a nearby neighbor or not. This leads to the idea of "equal representation" for each data point by a knot point. This means that each data point should be "close" to a knot point, and that each knot point should "represent" about the same number of data points. These two ideas are crucial to the knot selection algorithm. First, it is desirable to minimize the sum of the distances squared from each data point to the nearest knot point. Let the knot point locations be given by $(\hat{x}_j,\hat{y}_j)$, j=1, 2, ..., K. Then the function to be minimized is

$$GN^2 = \sum_{k=1}^{N} \min_j [(x_k-\hat{x}_j)^2+(y_k-\hat{y}_j)^2]$$

This process has a default Dirichlet tesselation with respect to the knot points, with each data point "belonging" to some knot point by virtue of the Dirichlet tile to which it belongs. When a data point lies on a tile boundary, some determination of which it belongs to, or whether it is shared must be assumed. Local minima for the above function are easily characterized: At a local minimum, each knot point $(\hat{x}_j,\hat{y}_j)$ is the centroid of the data points in its tile. This leads to a nice algorithm for iteration to a local minimum, by repeated computation of the centroid of the data points in the Dirichlet tiles.

This algorithm works very well for obtaining a local minimum of the function GN^2. Unfortunately the function is rife with local minima, so that finding a desirable one depends on the proper initial guess. Here the second idea regarding "equal representation" comes into play. Since each data point is

assumed equally important, it is reasonable to expect that the Dirichlet tile for each knot should contain about the same number of data points. This leads to a heuristic for a new initial guess at knot locations once a local minimum for GN^2 has been found. It is still considered desirable to be at a local minimum of GN^2, but the idea of finding a global minimum of GN^2 is abandoned for the "equal representation" idea. Once a local minimum has been found, a new measure of "goodness" is computed. Let N_j be the number of points in the Dirichlet tile for the j^{th} knot point $(\hat{x}_j, \hat{y}_j)$. Let

$$D = \sum_{j=1}^{K} (N_j - N/K)^2 \ ,$$

a measure of the "equal representation" for a particular knot configuration. It was then attempted to determine knot locations which achieve a local minimum of GN^2 and which also yield a small value, hopefully a minimum, of D.

The general idea of the algorithm is to "nudge" the knot locations from a local minimum of GN^2 toward a configuration with smaller D value. The rationale for this is to attempt to move the tile boundaries across data points, yielding a more equitable distribution. The search for the minimum of D could turn out to be rather extensive, and for a large number of points with a moderately large number of knot points, the computational effort can be excessive. End results are still somewhat dependent on the initial guess, although the results generally tend to look quite reasonable. The program incorporates the option of internally generated (quasi-gridded) or user input initial guesses.

Examples are given which illustrate rather well the ability of the scheme to select knot locations which reflect the underlying density of the data. Actual surface fitting and comparison with two other methods, the Laplacian smoothing splines of Wahba and Wendelberger, and the tensor product bicubic Hermite method due to Foley [18], are reported upon. One example illustrates the failure of the fitting scheme to accurately model the surface when the data density does not reflect the underlying behavior of the surface, as was assumed.

4.3 Subset Selection

To my knowledge, the first investigation into the use of a subset of scattered data points upon which to base an interpolant to be used as an approximation for the entire data set was by Pickrell [47]. The application guided many of the ideas involved in the thesis and they are not universally applicable. Pickrell's goal was to model underwater terrain from a large number of measured depths, which were quite accurate, the most important being those which were on ridges or other shallow areas, since the resulting approximation could be used to generate charts for navigation.

The idea was to select as small a subset of points as possible such that the interpolant for these points yielded a surface that satisfied a certain error tolerance at all the other data points. An iterative scheme was used. Beginning with an initial guess, either taken "uniformly" spaced over the region of interest, or by perusal of the data for "critical" points such as high and low values or areas of sharp gradients. Call the selec-

ted points the "model" points. The interpolant (the MQ method was used; parameter r=0 generally performed best) was constructed and the deviation at other data points computed. Based on this information, other points at which the deviation was large, or one from a group of nearby points where deviations of the same sign occurred, would be included in the set of model points. Points with small coefficients might be eliminated from the set of model points, as well. The investigation did not yield an algorithm suitable for approximation with no intervention by the user, since this was performed interactively by Pickrell. In the examples reported, the required number of model points was generally on the order of 10-20% of the total number of points. However, only limited consideration was given to the handling of very large data sets which would require local application of the ideas with a scheme for joining the pieces together.

These deficiencies and other matters were addressed by Schiro and Williams [52]. In addition to automating the model point selection process, he subdivided the region into kernel groups based on a measure of homogeneity of the data. As a starting point the region of interest was divided into a rectangular grid of cells of size equal to the minimum to be considered. The mean and standard deviation of the function values (again, ocean depth data) were computed for each cell. Then, the cells were considered in turn as a base cell, and contiguous cells (with larger coordinates) having mean values within one standard deviation of the mean for the base cell were combined to form a larger rectangular cell, when possible. This larger group of cells is called a kernel group. Thus, each kernel group in the

final subdivision was made up of one or more contiguous cells in the original subdivision, all of which have similar mean behavior.

The selection of model points for each kernel group is done without user intervention. The initial set is chosen based on deviation from the mean value. (Of course, if all points are within the tolerance of the mean value, the mean value is used as the approximation for the kernel group.) The idea is similar to Pickrell's: points with large deviation are selected to be added to the set of model points, with the proviso that points closer than a certain distance cannot be selected on the same iteration. This avoids the problem of adding several points very close together on the same iteration. The process is continued until the deviations are below a specified tolerance.

The overall surface is made continuous by blending adjacent surfaces when within a certain distance from boundaries of the kernel groups. This is done via Hermite cubics to obtain a smooth transition. The MQ method with r=0 was used to fit the differences, data minus mean value, and this was observed to have a beneficial effect in terms of the magnitude of the coefficients in the representation.

Another approach to subset selection was taken by Bozzini, deTisi, and Lenarduzzi [5]. Here an attempt was made to determine a subset of points to be used to compute the approximation by doing local computations to determine whether a particular point has a significant influence on defining the surface. A description of the ideas will be given. The first step is to partition the region of interest into (probably overlapping) regions of given shape (e.g., circular disks) by taking the

region R_i as large as possible so that

$$\frac{1}{\text{area}(R_i)}\int_{R_i} |f(\mathbf{x})-f_i|\, d\mathbf{x} \leq K_i, \text{ for some constant } K_i.$$

The value of K_i specifies a kind of homogeneity of $f(\mathbf{x})$ over R_i. Then, for a weighting function $\phi_i(\mathbf{x})$, let

$$\delta_i = \int_{R_i} |f(\mathbf{x})-f_i|\, \phi(\mathbf{x})\, d\mathbf{x} \Big/ \int_{R_i} \phi(\mathbf{x})\, dx$$

This value serves as measure of the level of homogeneity in the region R_i, weighted by ϕ. Then a measure of the behavior of $f(\mathbf{x})$ at point i relative to point j (point j also in R_i) is given by

$$s_{ij} = |f_i-f_j|/\delta_i \ , \ j \neq i.$$

These values are averaged over the points in R_i to obtain s_i. The value of s_i is a measure of the what the authors call the "importance" of the point i in the data set, and hence to the definition of the approximating surface. The integrals in the definition are approximated with the obvious quadratures in the application. The point with the largest corresponding value of s_i is chosen. The process can then be repeated from the computation of the s_i to obtain more points, or one can choose the subset with the largest s_i values from the initial calculation. According to the authors, the method is not to sensitive to deletion of a point from the set. Some examples are given to illustrate approximation of surfaces from subsets of a given set of points.

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