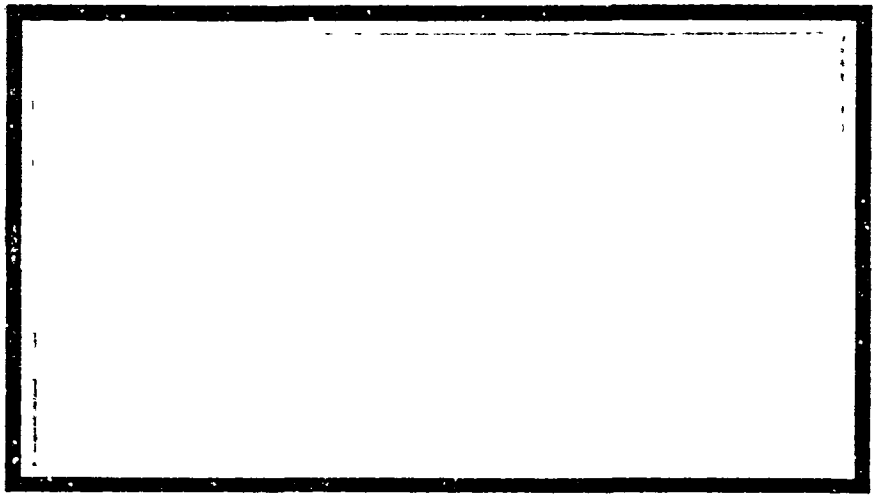

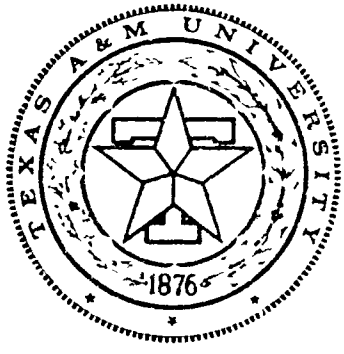

CENTER FOR APPROXIMATION THEORY

DEPARTMENT OF MATHEMATICS
TEXAS A&M UNIVERSITY
COLLEGE STATION, TEXAS 77843

PROCEEDINGS OF THE

NASA WORKSHOP ON SURFACE FITTING

Texas A&M University
College Station, Texas
May 17-19, 1982

Prepared for

Earth Resources Research Division
NASA/Johnson Space Center
Houston, Texas 77058

by

L. F. Guseman, Jr.
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under

NASA Contract NAS 9-16447

"Studies in Mathematical Pattern Recognition
and Image Analysis"

TABLE OF CONTENTS

Introduction

by

Larry L. Schumaker

On may 17-19, 1982, a workshop entitled "Surface Fitting" was held at Texas A&M University, College Station. The purpose of the workshop was to bring together leading experts from academia, industry, and government laboratories for an exchange of views and a discussion of the "state of the art." For a list of participants see pages 5-6.

The workshop began with an overview by R. P. Heydorn of NASA/Johnson Space Center, Houston, Texas. The purpose of the overview was to acquaint the participants with some mathematical/statistical problems within the AgRISTARS Program which may be amenable to investigations involving the use of surface-fitting techniques. In order to establish a framework for the workshop, Larry Schumaker presented a general survey of surface fitting and contouring in which he touched on a variety of local and global methods for both interpolation and approximation.

The program for the workshop included six invited lecturers (see the program on pages 3-5). Charles Lawson discussed the construction of a triangular grid on the sphere, and the computation of corresponding C^1 surfaces. R. E. Barnhill dealt with several schemes based on patches and blending. Rolland Hardy lectured on the multiquadric surfaces which he invented. Thomas Foley considered a three stage procedure which proceeds from scattered data to grid values using local least squares, then to a

bicubic B-spline interpolant, and finally uses Shepard's method to obtain an interpolant of the original data. Douglas Bates discussed smoothing splines and the method of generalized cross validation, with particular emphasis on computational methods. Rosemary Chang's talk dealt with several practical problems arising in Engineering.

In addition to the formal lectures, the program included a panel discussion involving everyone. We believe that the workshop gave all participants--the theoreticians, the practitioners, and the consumers--a better understanding of what methods and software are available, and of what needs to be done in the future.

Written versions of the lectures are included in this document. The talks elicited a great deal of discussion which we have not attempted to reproduce here. Finally, this document includes a computerized bibliography of surface fitting papers which Larry Schumaker has assembled at Texas A&M University. Additions and corrections to this bibliography would be greatly appreciated.

NASA WORKSHOP ON "SURFACE FITTING"

Texas A&M University
May 17-19, 1982
Room 206 Memorial Student Center

Monday, May 17

8:15 - 8:30	Coffee & Doughnuts
8:30 - 9:00	Introduction Larry F. Guseman, Jr., Texas A&M University
9:00 - 10:30	"Crop Proportion Estimation Problems in AgRISTARS" Richard P. Heydorn, NASA/Johnson Space Center
10:30 - 11:00	Coffee break
11:00 - 12:00	Overview Larry L. Schumaker, Texas A&M University
12:00 - 1:30	Lunch
1:30 - 2:30	"C1 Surface Interpolation for Scattered Data on a Sphere" Chuck Lawson, Jet Propulsion Labs, Cal Tech
2:30 - 3:00	Coffee break
3:00 - 4:00	"Computer-Aided Surface Representation" Bob Barnhill, University of Utah

Tuesday, May 18

8:15 - 8:30	Coffee & Doughnuts
8:30 - 9:30	"Application of Surface Modeling Techniques to Engineering Problems" Rosemary E. Chang, Sandia National Labs
9:30 - 10:30	"Surface Fitting with Biharmonic and Harmonic Models" Rolland L. Hardy, Iowa State University
10:30 - 11:00	Coffee break
11:00 - 12:00	"BSPLASH: A Three-Stage Surface Interpolant to Scattered Data" Tom Foley, California Polytechnic
12:00 - 1:30	Lunch

Workshop on "Surface Fitting"

1:30 - 2:30	Douglas Bates, University of Wisconsin--Madison
2:30 - 3:00	Coffee break

Dinner at Larry Guseman's cabin

Wednesday, May 19

8:15 - 8:30	Coffee & doughnuts
8:30 - 10:00	Panel discussion: Research Issues in Surface Fitting Applicable to NASA
10:00 - 10:30	Coffee Break
10:30 - 12:00	Panel discussion, continued.

NASA WORKSHOP ON SURFACE FITTING

May 17-19, 1982

Participants and Other Attendees:

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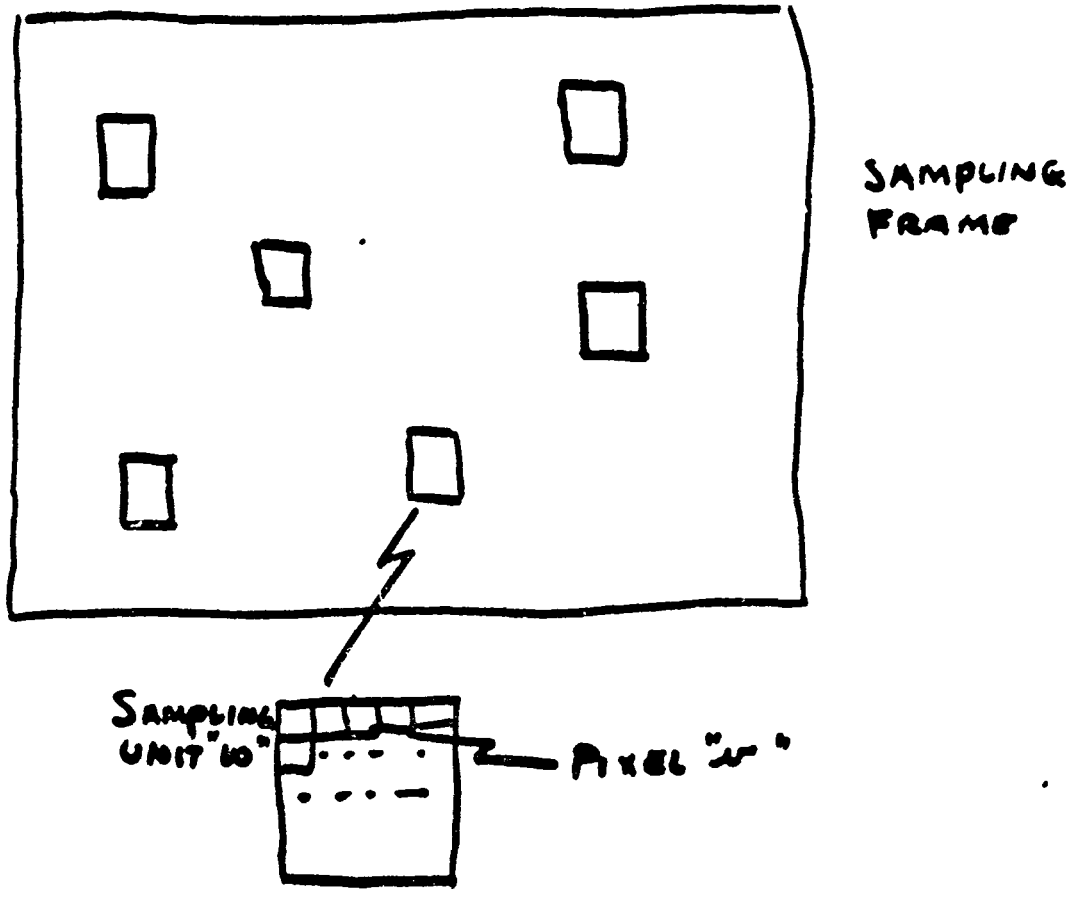
University of California
Santa Barbara, CA 93106

Crop Proportion Estimation Problems in AgRISTARS

Richard P. Heydorn
NASA/Johnson Space Center
Earth Observation Division

Workshop on Surface Fitting
May 17, 1982

NOTATION



$\Theta(x;\omega) \in \{0,1\}$ ~ TRUE LABEL OF A PIXEL

$\vec{z}(x;\omega) \in \mathbb{R}^n$ ~ VECTOR OF SPECTRAL MEASUREMENTS

$\Phi(\vec{z}(x;\omega)) \in \{0,1\}$ ~ CLASSIFIER

CLASSIFICATION

EXAMPLE: BAYES RULE

LET f_1 ~ CONDITIONAL DENSITY OF "CROP OF INTEREST"

f_0 ~ CONDITIONAL DENSITY OF "OTHER"

y ~ PRIOR FOR CROP OF INTEREST

$\phi(z) = 1$ IF

$$y f_1(z) > (1-y) f_0(z)$$

$\phi(z) = 0$ IF

$$y f_1(z) \leq (1-y) f_0(z)$$

MAXIMUM LIKELIHOOD RULE

SAME AS BAYES RULE BUT USE $y = \frac{1}{2}$
(i.e. IGNOR PRIORS)

BIAS

CLASSIFY A SAMPLING UNIT AND COUNT PIXELS FOR WHICH $\Phi(z)=1$ TO ESTIMATE PROPORTION OF THE CROP OF INTEREST

FOR SAMPLING UNIT "ω"

$$X(\omega) = \frac{1}{N}\sum_{i=1}^{N} \Phi(z_i(\omega)) \doteq P_r(\Phi(z(\omega))=1)$$

LET

$$Y(\omega) = \frac{1}{N}\sum_{i=1}^{N} \Theta_i(\omega) \doteq P_r(\Theta(\omega)=1) \text{ TRUE PROP.}$$

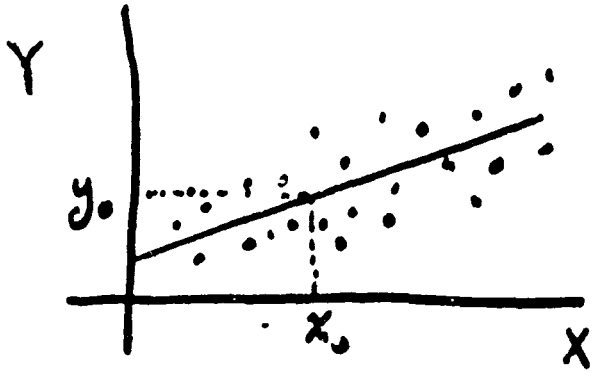
NOW, (FOR LARGE N)

$$X(\omega) = P_r(\Phi(z)=1 \mid \Theta=0)\,(1-Y(\omega)) + P_r(\Phi(z)=1 \mid \Theta=1)\,Y(\omega)$$

$$\text{BIAS} = X(\omega)-Y(\omega) = \underbrace{P_r(\Phi(z)=1 \mid \Theta=0)}_{\text{COMMISSION ERROR}}(1-Y(\omega)) - \underbrace{P_r(\Phi(z)=0 \mid \Theta=1)}_{\text{OMISSION ERROR}}\,Y(\omega)$$

Regression Estimators

In Domestic Applications Ground Samples Are Available and ∴ can be used To "UNBIAS" A Classifier Derived Estimate



Model

$$Y = a + GX + \varepsilon$$

For $a = E(Y) - GE(X)$

$$E(Y) = Y + G(E(X) - X) - \varepsilon$$

$$\widehat{E(Y)} = Y + G(E(X) - X)$$

$$VAR(\widehat{E(Y)}) = VAR(Y)(1 - R^2)$$

CLASSIFIER DESIGN

PROBLEM: HOW TO DESIGN THE CLASSIFIER SO THAT THE REGRESSION FUNCTION

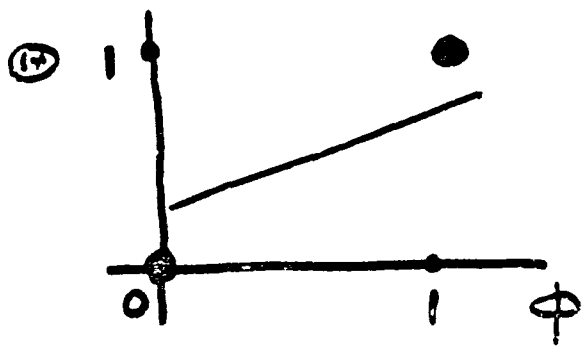
$$E(Y|X)$$

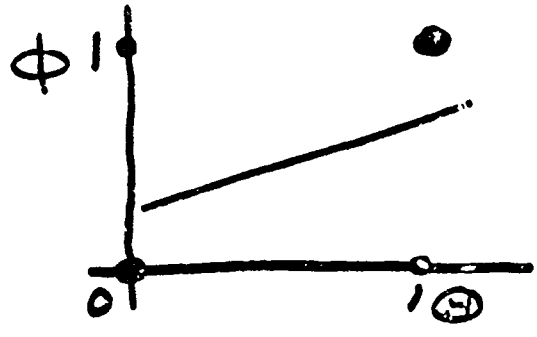
OR

$$E(X|Y)$$

WILL ASSUME A GIVEN FORM?

TWO POINT MODEL





$$\Phi = \alpha_\omega + \beta_\omega \Phi(x) + \zeta$$

WHERE

$$\alpha_\omega = P_r(\Phi = 1 \mid \Phi(x) = 0, \Delta = \omega)$$

$$\beta_\omega = P_r(\Phi = 1 \mid \Phi(x) = 1, \Delta = \omega)$$

$$\Phi(x) = \gamma_\omega + \delta_\omega \Phi + \eta$$

WHERE

$$\gamma_\omega = P_r(\Phi(x) = 1 \mid \Phi = 0, \Delta = \omega)$$

$$\delta_\omega = P_r(\Phi(x) = 1 \mid \Phi = 1, \Delta = \omega)$$

LET $A_x = \{\omega : X(\omega) = x\}$

$B_y = \{\omega : Y(\omega) = y\}$

THEOREM

$$E(Y|X) = \bar{\alpha}_X + \bar{\beta}_X X$$

$$E(X|Y) = \bar{\gamma}_Y + \bar{\delta}_Y Y$$

WHERE

$$\bar{\alpha}_X = Pr(\Theta = 1 \mid \Phi(\delta) = 0, \Delta \in A_X)$$

$$\bar{\beta}_X = Pr(\Theta = 1 \mid \Phi(\delta) = 1, \Delta \in A_X) - \bar{\alpha}_X$$

$$\bar{\gamma}_Y = Pr(\Phi(\delta) = 1 \mid \Theta = 0, \Delta \in B_Y)$$

$$\bar{\delta}_Y = Pr(\Phi(\delta) = 1 \mid \Theta = 1, \Delta \in B_Y) - \bar{\gamma}_Y$$

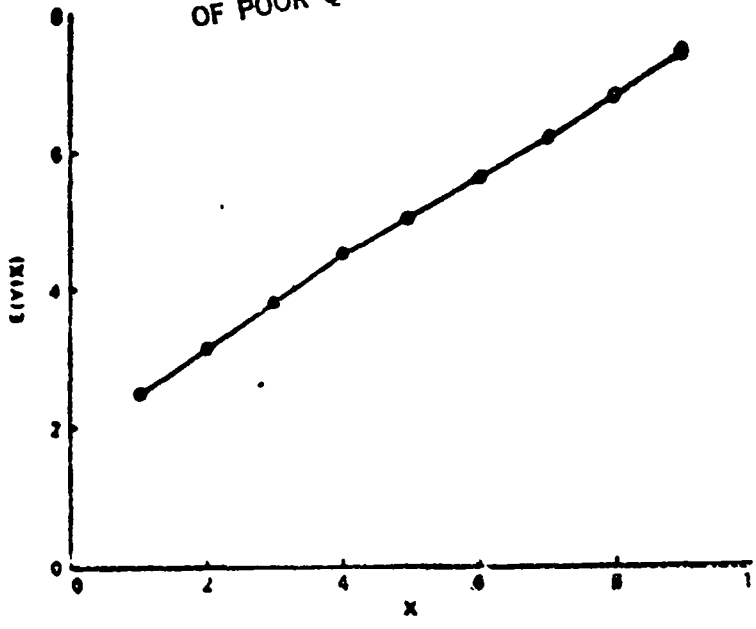


Figure 1(a) – E(Y|X FOR THE BAYES CLASSIFIER

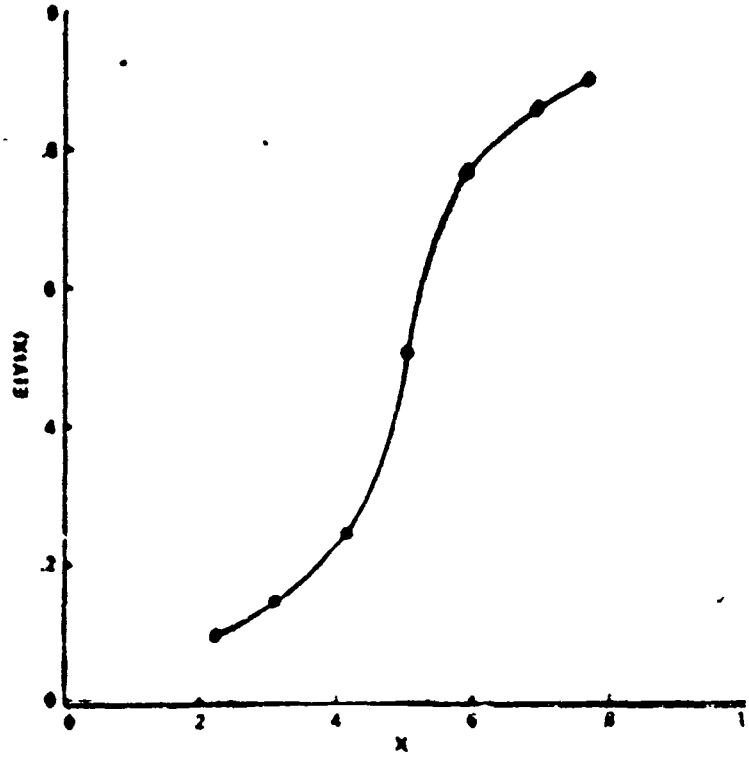


Figure 1(b) - E(Y|X) FOR THE MAXIMUM LIKELIHOOD CLASSIFIER

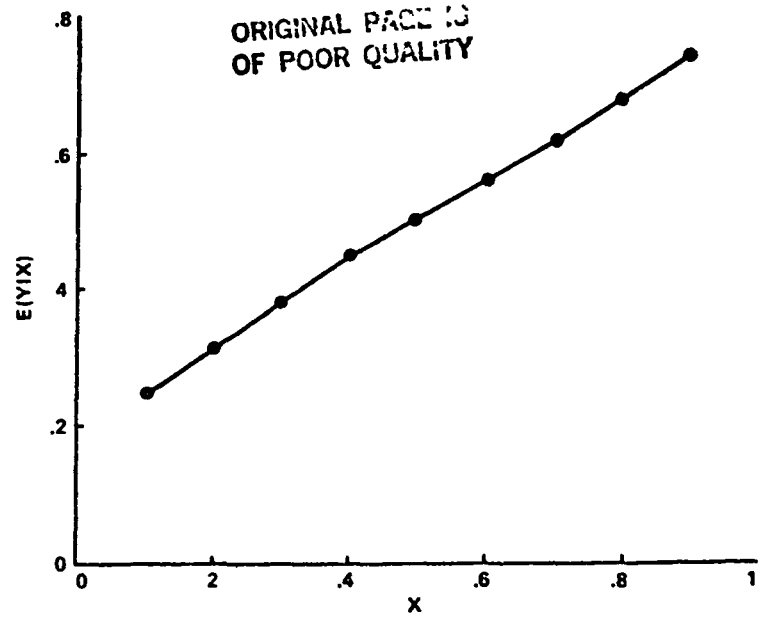


Figure 1(a) – E(YIX FOR THE BAYES CLASSIFIER

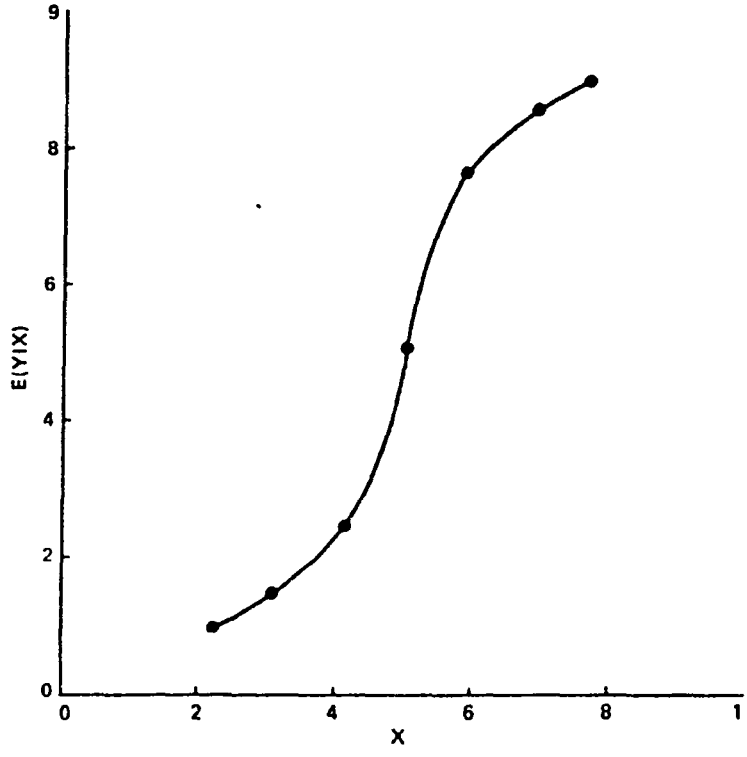


Figure 1(b) – E(YIX) FOR THE MAXIMUM LIKELIHOOD CLASSIFIER

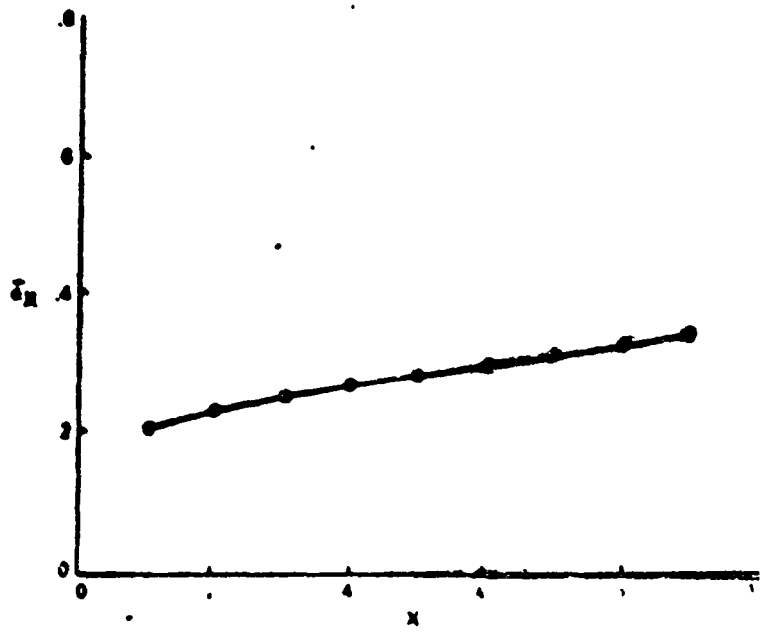


Figure 1(c) – $\bar{a}_X$ FOR THE BAYES CLASSIFIER

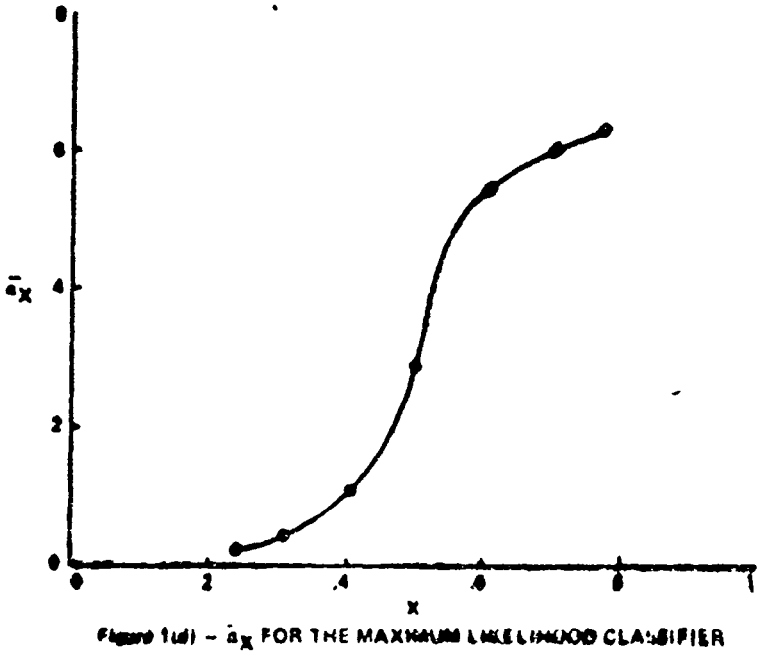


Figure 1(d) – $\bar{a}_X$ FOR THE MAXIMUM LIKELIHOOD CLASSIFIER

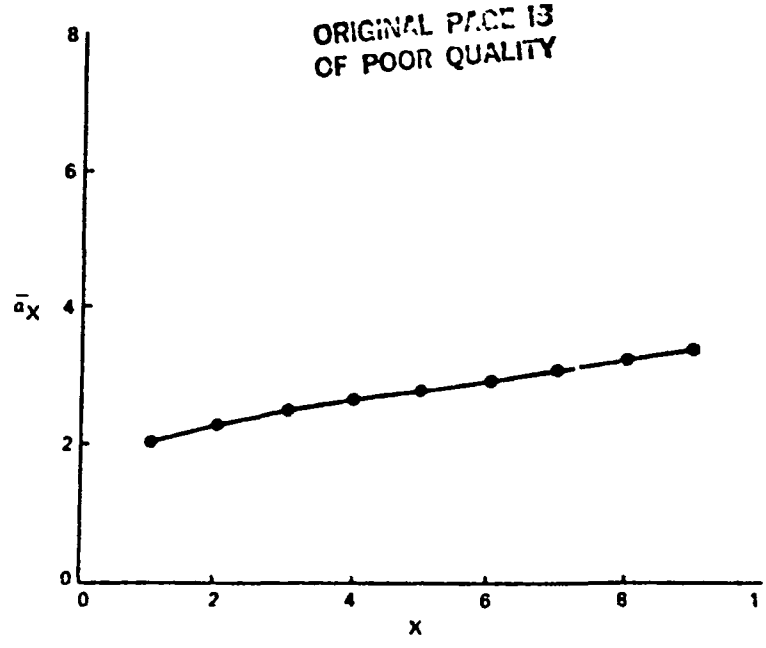


Figure 1(c) – $\bar{a}_X$ FOR THE BAYES CLASSIFIER

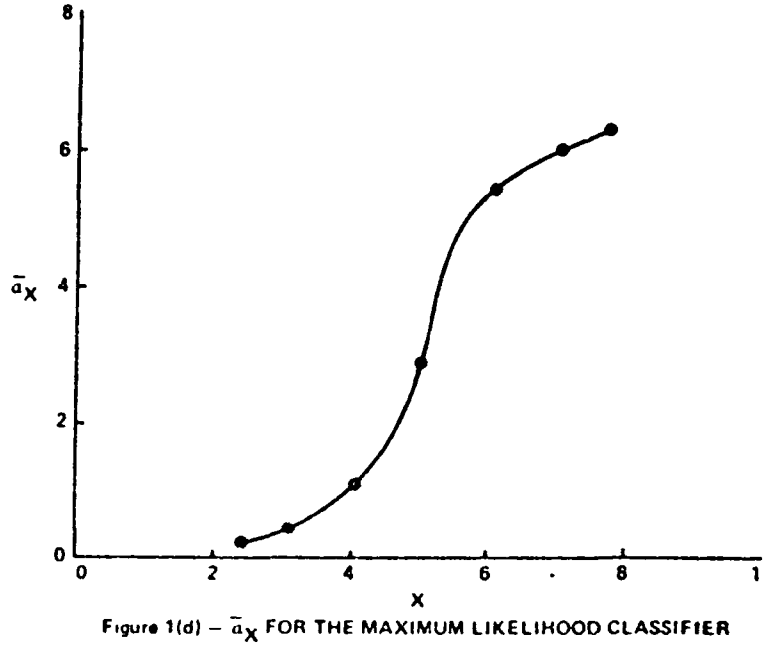


Figure 1(d) – $\bar{a}_X$ FOR THE MAXIMUM LIKELIHOOD CLASSIFIER

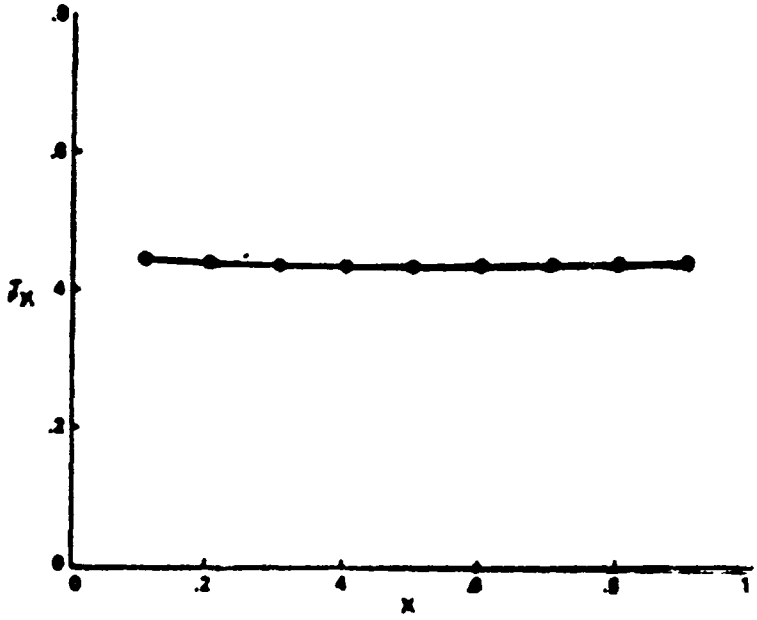


Figure 1(e) – $\bar{\beta}_X$ FOR THE BAYES CLASSIFIER

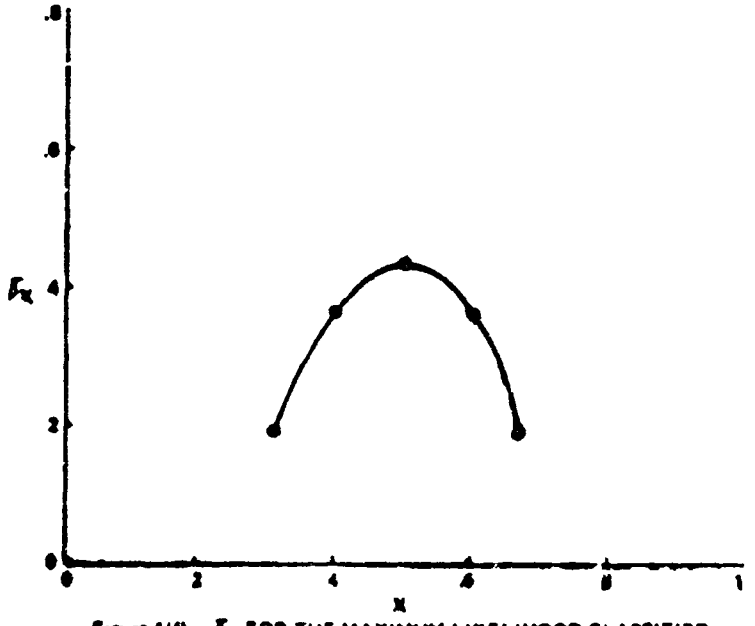


Figure 1(f) – $\bar{\beta}_X$ FOR THE MAXIMUM LIKELIHOOD CLASSIFIER

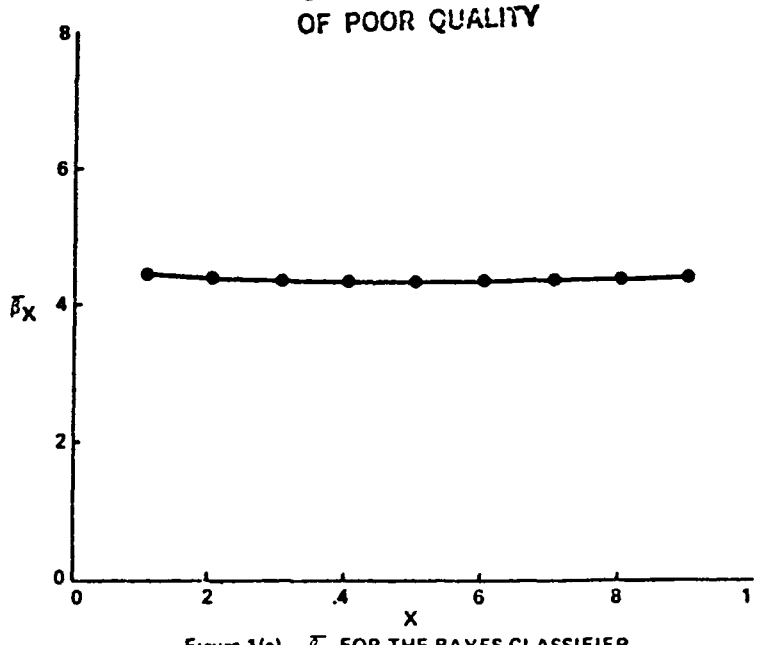


Figure 1(e) – $\bar{\beta}_X$ FOR THE BAYES CLASSIFIER

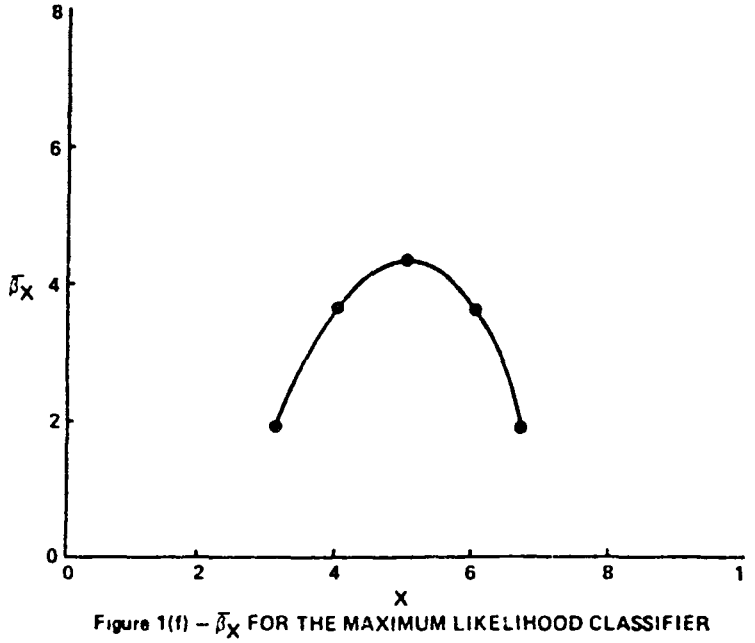


Figure 1(f) – $\bar{\beta}_X$ FOR THE MAXIMUM LIKELIHOOD CLASSIFIER

Sampling Efficiency

$$VAR\left(E(\hat{Y})\right) = VAR(Y)\left(1-R^2\right)$$

For $\bar{\alpha}_x$, $\bar{\beta}_x$ constant

$$R^2 = \left(1-\Psi_o-\Psi_c\right)^2 \frac{\pi(1-\pi)}{\lambda(1-\lambda)} \frac{\rho_1}{\rho_2}$$

$\Psi_o \sim$ omission Error

$\Psi_c \sim$ Commission Error

$\pi = Pr(\Phi=1)$

$\lambda = Pr(\phi(\vec{x})=1)$

$\rho_1 = VAR(X)/\lambda(1-\lambda)$

$\rho_2 = VAR(Y)/\pi(1-\pi)$

OPEN PROBLEMS

OPTIMUM CLASSIFIER DESIGN FOR $E(Y|X)$?

OPTIMUM CLASSIFIER DESIGN FOR $E(X|Y)$?

OPTIMUM CHOICE; $E(Y|X)$ OR $E(X|Y)$?

Direct Proportion Estimation

Mixture Model

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

f_i ~ Likelihood of Crop i

λ_i ~ Proportion of Crop i

M ~ # of Crop (Material) Classes

f ~ Mixture Density

Problems

- Representation
- Labeling
- Parameter Estimation

PARAMETER ESTIMATION

EST. OF $\lambda_i, \mu_i, \Sigma_i$ IN THE MODEL

$$f(\cdot) = \sum_{i=1}^{M} \lambda_i N(\cdot; \mu_i, \Sigma_i)$$

MAX. LIKELIHOOD EST. GIVEN iid SAMPLE

$Z_1, Z_2, \ldots, Z_m$.

$$\lambda_i^{(k+1)} = \frac{1}{m} \sum_{j=1}^{m} \frac{\lambda_i^{(k)} N(z_j; \mu_i^{(k)}, \Sigma_i^{(k)})}{f^{(k)}(z_j)}$$

$$\mu_i^{(k+1)} = \frac{\sum_{j=1}^{m} z_j \frac{N(z_j; \mu_i^{(k)}, \Sigma_i^{(k)})}{f^{(k)}(z_j)}}{\sum_{j=1}^{m} \frac{N(z_j; \mu_i^{(k)}, \Sigma_i^{(k)})}{f^{(k)}(z_j)}}$$

$$\Sigma_i^{(k+1)} = \frac{\sum_{j=1}^{m} (z_j - \mu_i^{(k+1)})(z_j - \mu_i^{(k+1)})' \frac{N(z_j; \mu_i^{(k)}, \Sigma_i^{(k)})}{f^{(k)}(z_j)}}{\sum_{j=1}^{m} \frac{N(z_j; \mu_i^{(k)}, \Sigma_i^{(k)})}{f^{(k)}(z_j)}}$$

Estimation of M

1. Akaike Information Criterion (AIC)

$$AIC = -2\, L(\hat{\xi}) + 2\frac{t}{m}$$

$L(\hat{\xi})$ = value of Log Likelihood Eval. at the Max. Likelihood Est. $\hat{\xi}$

t = # of Free Parameters

m = Sample Size

2. Trigonometric Moments

Theorem (Carathéodory)

$C_1, C_2, \ldots, C_m$ complex constants Not all zero, $m \geq 1$. There Exists an Integer M ($\leq m$) and Constants ρ_k, ε_k, $k = 1, 2, \ldots, M$ such that $\rho_k > 0$, $|\varepsilon_k| = 1$, $\varepsilon_k \neq \varepsilon_\ell$, $k \neq \ell$

$$C_\nu = \sum_{k=1}^{M} \rho_k \varepsilon_k^\nu$$

- M and ρ_k are unique

To Apply The Theorem Take The Fourier Transform of

$$f(\cdot) = \sum_{k=1}^{M} \lambda_k N(\cdot; \mu_k, \sigma)$$

i.e.

$$\psi(\omega) = \sum_{k=1}^{M} \lambda_k e^{i\mu_k\omega - \frac{\sigma^2\omega^2}{2}} \quad ; \; i = \sqrt{-1}$$

$$\underbrace{e^{\frac{\sigma^2\omega^2}{2}}\psi(\omega)}_{c_\omega} = \sum_{k=1}^{M} \underbrace{\lambda_k}_{\rho_k} \underbrace{\left(e^{i\mu_k}\right)^{\omega}}_{\varepsilon_k^{\omega}}$$

$M, \mu_k, \lambda_k; k = 1, 2, \ldots, M$ obtained from

$$\begin{pmatrix} 1 & c_1 & c_2 & \cdots & c_M \\ \bar{c}_1 & 1 & c_1 & \cdots & c_{M-1} \\ \vdots & & & & \\ \bar{c}_M & \bar{c}_{M-1} & \cdots & \cdots & 1 \end{pmatrix}$$

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D2

FITTING SURFACES TO SCATTERED DATA

Larry L. Schumaker

This paper is a survey of a variety of numerical methods for fitting a function to data given at a set of points scattered throughout a domain in the plane. We discuss four classes of methods: (1) global interpolation, (2) local interpolation, (3) global approximation, and (4) local approximation. We also discuss two-stage methods and contouring. The surfaces constructed will include polynomials, spline functions, and rational functions, among others.

1. Introduction

Our aim is to survey methods for solving the following problem.

PROBLEM 1.1. Let D be a domain in the (x,y)-plane, and suppose F is a real-valued function defined on D. Suppose we are given the values $F_i = F(x_i,y_i)$ of F at some set of points (x_i,y_i) located in D, i = 1,2,...,N. Find a function f defined on D which reasonably approximates F.

This problem is, of course, precisely the problem of fitting a surface to given data. In many cases the domain D is a rectangle and the data points lie on a rectangular grid. There are, however, many practical problems (see the following section for some specific examples), where D is of unusual shape and where the data points are irregularly scattered throughout D. Thus, while we shall pay some attention to special methods for regularly spaced data, we are actually more interested in the general case.

There are basically two approaches to handling Problem 1.1. First, we may try to construct a function f which interpolates

the data exactly; i.e., such that

(1.1) $f(x_i,y_i) = F_i, \quad i = 1,2,\ldots,N.$

This approach may be desirable when the function values at the data points are known to high precision and where it is highly desirable that these values be preserved by the approximating function.

The second approach involves constructing f which only approximately fits the data. This may be regarded as data smoothing and will be desirable when (as is often the case) the data are subject to inaccurate measurement or even errors. The question of whether interpolation or approximation should be used will not be discussed further here--this is a problem which must be settled for the individual problem at hand.

In discussing Problem 1.1, it will be convenient to make a further distinction between those methods which are local in character (i.e., where the value of the constructed surface f at the point (x,y) depends only on the data at relatively nearby points) and those methods which are global in nature. Thus, we discuss four categories of methods in sections 3-6: (1) global interpolation, (2) local interpolation, (3) global approximation, and (4) local approximation. In each of these sections we further subdivide the material according to the type of functions being used and the type of data (scattered or not) for which the method is suitable.

In discussing methods which apply only to special arrangements of data points, we have two objectives in mind. First, the methods are of interest in their own right. More importantly in terms of Problem 1.1, however, such methods can also be used in two-stage processes in which we first construct a surface g based on the scattered data, and then use g to generate regular data for the construction of another (perhaps smoother or more convenient) surface f. Such two-stage methods

will be discussed (along with several examples) in more detail in section 7.

For many of the methods based on regular data and some of those for scattered data, error bounds are available to indicate how well smooth functions are approximated by the surface constructed. We do not have space to go into the extensive literature on error bounds. A simple test of how well a method will approximate smooth functions is, however, provided by its ability to reproduce polynomial surfaces exactly (that is, if F is a polynomial in x and y up to a certain degree, then the surface f is identically equal to F). For many of the methods we will be able to indicate the corresponding degree of exactness.

In many of the applications of surface-fitting techniques (cf. the examples in section 2), the ultimate aim is to use the data to construct a contour map of the unknown function. Since F is known only at the data points, we must be content to construct a contour map for one of our fitted surfaces. In section 8 we discuss some approaches to accomplishing this numerically.

We close this introduction with a disclaimer--this survey does not include all possible methods for fitting surfaces to scattered data. For example, we have not discussed Fourier series methods, spatial filtering, and other such related statistical techniques. In addition, the set of references for those methods which we have discussed are also not complete. My original intention was to compile as complete a bibliography as possible, but the sheer bulk of relevant papers and my inability to locate all of them convinced me to settle for less. I have opted to quote a fairly representative list of papers, including several other surveys. Further references can be found by consulting these. I shall be very happy to receive information on references and methods I have overlooked.

2. Examples

In this section we shall quote several explicit examples of Problem 1.1 to emphasize the fact that unusually shaped regions and scattered data do arise frequently in practice.

EXAMPLE 2.1. Petroleum exploration. In exploring for petroleum, the contours of various underground layers of sandstone, shale, limestone, etc. can be important indicators of possible oil fields. Frequently, data on such layers is available from exploratory wells, which, however, have most likely been drilled at locations scattered randomly throughout some geographical region of interest. To quote a specific example, Robinson, Charlesworth, and Ellis [166] consider precisely this problem for some data obtained from 7,500 wells drilled in Alberta. For another example of this type, see Whitten and Koelling [208].

Problems similar to that mentioned in Example 2.1 arise frequently in cartography and submarine topography where the measurements represent actual elevations. In some cases the measurements must be taken from photographs or from sonar measurements and are usually subject to some measurement error (eg. see Kubik [125] for a discussion of photogrammetry).

EXAMPLE 2.2. Geological maps. There are a great many problems in Geology and the earth sciences in which the data arises from some other function of location besides actual elevations. For example, some geological variables of interest might include concentrations of various chemicals, specific gravity, electrical resistivity, grain size, texture, optical properties, isotope ratios, etc. To quote a specific example, Bhattacharyya [21, 22] discusses methods for fitting a surface to measurements (taken by airborne sensors) of magnetic potentials over a certain portion of the Yukon. See also Bhattacharyya and Raychaudhuri [23] and Crain and Bhattacharyya [61].

The importance of surface-fitting methods in the earth sciences can be judged by the large number of papers in the area relating to various fitting methods. For a further list of problems and a discussion of some of the methods which have been applied, see the books of Bohrenberg and Giese [31], Chorley [51], David [62], Harbaugh and Merriam [98], and Merriam [140]. Recent survey papers include Whitten [203, 205] and Whitten and Koelling [207]. To add just a few more of the papers in the geological literature dealing with surface fitting to our list, we mention Anderson [7], Grant [91], Hessing, Lee, and Pierce [114], Holroyd and Bhattacharyya [115], Kubik [123, 125], Norcliffe [151], Reilly [162], Whitten [200, 201, 204], and Whitten and Koelling [206].

EXAMPLE 2.3. Heart potentials. In order to diagnose certain abnormal heart conditions, it is desired to make a series of several hundred contour maps of the heart potential field at time steps of 1/100 of a second throughout a heart beat. Data on these heart potentials can be obtained by fitting the patient with a shirt containing probes. Because of body geometry, when this shirt is flattened out it takes the nonrectangular form illustrated in Figure 1. Although the probes could be arranged fairly regularly in this domain, because of the added signifi-

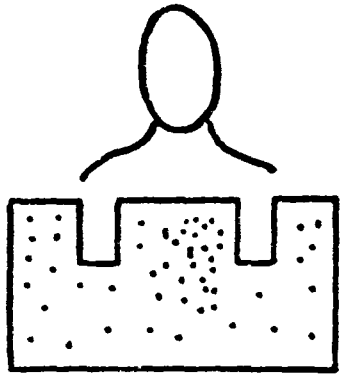

Figure 1. Heart Potential Measurements

cance of frontal measurements, in practice more probes are fitted there than in the back. This example was brought to my attention by Ms. Patrizia Ciarlini of Rome.

Potential fields arise in many other applications. We have already mentioned Geology in Example 2.2. For some examples in modelling plasmas see Buneman [40]. The problem arises in Biersack and Fink [24] in experimentally studying crystal structure using neutron bombardment. Data from waveform distortion in electronic circuits can be found in Akima [5, 6].

3. Global interpolation methods

In this section we outline several methods for solving the interpolation problem (1.1).

3.1 Polynomial interpolation. (Scattered data). The general theory of finite dimensional interpolation is, of course, very well known (e.g., see Davis [63]). Briefly, if $\{\phi_i\}_1^N$ are N functions defined on the domain D, then the function

$$(3.1) \quad f(x,y) = \sum_{j=1}^{N} a_j \phi_j(x,y)$$

will satisfy (1.1) if and only if $\{a_j\}_1^N$ is a solution of the linear system

$$(3.2) \quad \sum_{j=1}^{n} a_j \phi_j(x_i,y_i) = F_i, \quad i = 1,2,\ldots,N.$$

This system has a (unique) solution for arbitrary choices of data precisely when it is nonsingular. This depends on the choice of functions $\{\phi_j\}_1^N$ and the location of the data points.

To illustrate this method, we may choose the $\{\phi_j\}_1^N$ to be polynomials in x and y. Given N, there is some leeway in the choice of which powers of x and y to use. For example, with N = 3 one could use the functions 1, x, y or possibly the functions 1, x^2, y^2, etc. When N is of the form N =

$(d+1)(d+1)$, we might use the functions

$$\{\phi_j(x,y)\}_1^N = \{x^\nu y^\mu\}_{\nu=0,\mu=0}^{d,d}$$

As simple as this sounds, there are some serious difficulties with polynomial interpolation of scattered data. For openers, it is not so easy to guarantee that the system (3.2) is nonsingular. To give a very simple example, consider the case $N = 3$ with the functions $1, x, y$. If the three data points happen to lie on a line, then (3.2) will in fact be singular. Even when (3.2) is nonsingular, it will often be the case (at least if N is moderately large) that the system will be ill-conditioned. Finally, as is well known, polynomials of even moderate degree exhibit a considerable oscillatory character, and the resulting surface (even though it is C^∞) is often too undulating to be acceptable. The general problem of polynomial interpolation to scattered data is not usually treated in Numerical Analys's and Approximation Theory books (see, however, Kunz [126], Prenter [157], and Steffenson [186]). Some papers dealing with the question include Guenther [93], Thatcher [189], Thatcher and Milne [190], and Whaples [197]. Assuming the interpolant exists, error bounds have been studied in Ciarlet and Raviart [52-55].

Let

$$(3.3)\quad \mathcal{P}_{m,n} = \text{span}\,\{x^\nu y^\mu\}_{\nu=0,\mu=0}^{m,n}$$

be the space of polynomials of degree m in x and of degree n in y. This linear space is of dimension $(m+1)(n+1)$ and is, in fact, the tensor product of the linear spaces $\mathcal{P}_m$ and $\mathcal{P}_n$. It is perhaps of interest to note that there always exists a (usually nonunique) polynomial $p \in \mathcal{P}_{N,N}$ which solves the interpolation problem (1.1), no matter how the data points are positioned, see Prenter [158].

3.2 Polynomial interpolation (gridded data). We begin this subsection by defining what we mean by gridded data. Let

$$H = [a,b] \times [c,d] \tag{3.4}$$

be a rectangle, and let

$$\begin{aligned} a = x_0 < x_1 < \ldots\ldots < x_{k+1} = b \\ c = y_0 < y_1 < \ldots\ldots < y_{\ell+1} = d. \end{aligned} \tag{3.5}$$

We suppose now that F is a function defined on H, and that we have the values of F at the corner points of the rectangular grid defined by (3.5); i.e.,

$$F_{ij} = F(x_i,y_j), \quad \begin{matrix} i = 0,1,\ldots,k+1 \\ j = 0,1,\ldots,\ell+1. \end{matrix} \tag{3.6}$$

This is a total of $N = (k+2)(\ell+2)$ data points.

It is quite easy to show that there exists a unique polynomial p in the class $\mathcal{P}_{k+1,\ell+1}$ (cf. the definition (3.3)) which interpolates the gridded data given in (3.4)-(3.6). In fact, p can be written down explicitly in terms of the one-dimensional Lagrange polynomials as

$$p(x,y) = \sum_{i=0}^{k+1} \sum_{j=0}^{\ell+1} F_{ij} L_i(x) \tilde{L}_j(y), \tag{3.7}$$

where the $\{L_i(x)\}_0^{k+1}$ and $\{\tilde{L}_j(y)\}_0^{\ell+1}$ are the usual one-dimensional Lagrange polynomials associated with the interpolation points $\{x_i\}_0^{k+1}$ and $\{y_j\}_0^{k+1}$, respectively. Interpolation of gridded data by polynomials has been discussed in various books and papers--we do not bother with a long list. See e.g. Prenter [157] or Steffenson [186]. More recently, there has been considerable work on Hermite and osculatory interpolation in several variables; see e.g. Ahlin [3], Haussman [99,101,102], and Salzer [168-170].

3.3 Shepard's method. In this subsection we discuss a method of Shepard [180] and some modifications of it. The method applies to arbitrarily spaced data, and the interpolating function can be written down explicitly.

Let ρ be some metric in the plane, for example the usual distance metric. Given a point (x,y), let $r_i = \rho((x,y),(x_i,y_i))$ for $i = 1,2,\ldots,N$. Let $0 < \mu < \infty$. Then Shepard's interpolation formula is defined by

$$(3.8)\quad f(x,y) = \begin{cases} \left(\sum_{i=1}^{N} \frac{F_i}{r_i^{\mu}}\right) \Big/ \left(\sum_{i=1}^{N} \frac{1}{r_i^{\mu}}\right), & \text{when } r_i \neq 0, \text{ all } i \\ F_i, & \text{when } r_i = 0. \end{cases}$$

The formula (3.8) is defined for all points (x,y) in the plane R^2. It is clear from the definition that it interpolates the values F_i at the data points (x_i,y_i), $i = 1,2,\ldots,N$. The value of $f(x,y)$ at nondata points is obtained as a weighted average of all the data values, where the i^{th} measurement is weighted according to the distance of (x,y) from the point (x_i,y_i).

We shall briefly recount some of the properties of Shepard's formula. First, by converting all of the terms to a common denominator, it can be shown that

$$(3.9)\quad f(x,y) = \sum_{i=1}^{N} F_i A_i(x,y),$$

where

$$(3.10)\quad A_i(x,y) = \frac{\prod_{\substack{j=1 \\ j\neq i}}^{N} [r_j(x,y)]^{\mu}}{\sum_{k=1}^{N} \sum_{\substack{\ell=1 \\ \ell\neq k}}^{N} [r_\ell(x,y)]^{\mu}}, \quad i = 1,2,\ldots,N.$$

These functions satisfy

(3.11) $A_i(x_j,y_j) = \delta_{ij}, \quad i,j = 1,2,\ldots,N.$

The representation (3.9) is numerically more stable than the original formula (3.8).

In view of its definition, we see that the function $f(x,y)$ constructed by Shepard is not a simple polynomial or rational function. It is clear, however, that except for the points (x_i,y_i), it is analytic everywhere in the plane. Its behavior in the vicinity of the data points (x_i,y_i) depends on the size of μ. It can be shown that for $0 < \mu \leq 1$, f has cusps at these points. For $1 < \mu$, f has flat spots at the data points (i.e., the partial derivatives vanish there). We also observe the interesting property that

(3.12) $$\min_{1\leq i\leq N} F_i \leq f(x,y) \leq \max_{1\leq i\leq N} F_i.$$

We may also note that if the data came from a constant function, i.e., $F_i = c$, $i = 1,2,\ldots,N$, then f is also the constant function $f \equiv c$.

We now comment on the choice of μ. To get smooth surfaces without cusps, it is desirable to take $1 < \mu$. On the other hand, if μ is relatively large, then the surface tends to become very flat near the data points and consequently quite steep at points in between. Experiments (cf. Gordon and Wixom [90], Poeppelmeir [155], and Shepard [180]) seem to indicate that a choice of $\mu = 2$ is perhaps a good tradeoff. ([155] contains several examples showing the behavior as a function of μ.)

There are several drawbacks to Shepard's method (3.8), as pointed out by Shepard [180] himself. First, if N is large, then there is a very considerable amount of calculation involved in evaluating $f(x,y)$ at a particular point. Secondly, the weights are assigned on the basis of the distance of points from (x,y) only, not their direction. Finally, the flat spots

in the neighborhood of the data points is somewhat disturbing. The first of these objections can be met by defining a local version of the formula, which we shall do in section 4.5. It is possible to construct an analogous formula which accounts for direction. For details, see Shepard [180]. Finally, we briefly discuss handling the flat spots.

Suppose in addition to the function values F_i at each point (x_i,y_i) we also have estimates FX_i and FY_i of $F_x(x_i,y_i)$ and $F_y(x_i,y_i)$. Then we may consider the function

$$(3.13)\quad f(x,y) = \sum_{i=1}^{N} A_i(x,y)\,[F_i + (x-x_i)FX_i + (y-y_i)FY_i].$$

It is easily checked that this function also interpolates, and that

$$(3.14)\quad f_x(x_i,y_i) = FX_i \qquad f_y(x_i,y_i) = FY_i, \quad i = 1,2,\ldots,N.$$

This property may be expressed in the assertion that if the data F_i, FX_i, FY_i came from a plane surface F, then f will exactly reproduce this surface. To use formula (3.13) in practice on the data-fitting Problem 1.1, we have to carry out a two-stage approximation process in which the first stage consists of some method for estimating the slope at each of the data points.

It might be of practical interest in some cases to construct still a more sophisticated version of Shepard's formula which would exactly reproduce higher-order polynomial surfaces. One approach to doing this is to use the following lemma.

LEMMA 3.1. (Barnhill [15]). Let P and Q be linear projections of some linear space of functions $\mathcal{F}$ into itself. Suppose that Q exactly reproduces the linear subspace $E \subset \mathcal{F}$; i.e.,

$$(3.15)\quad Qp = p, \quad \text{all} \quad p \in E.$$

In addition, suppose that $\{\lambda_i\}_1^m$ is a set of linear functionals on $\mathcal{F}$, and that

(3.16) $\lambda_i Pf = \lambda_i f$, all $f \in \mathcal{F}$, $i = 1,2,\ldots,m$.

Then the Boolean sum projector

(3.17) $P \oplus Q = P + Q - PQ$

enjoys the function precision of Q (i.e., reproduces E) and the interpolation properties of P (i.e., (3.16) also holds for $P \oplus Q$).

This result permits the construction of interpolation schemes using Shepard's formula which reproduce higher-order surfaces. For an example, see Poeppelmeir [155] where Shepard's formula is combined with a certain local interpolation scheme which reproduces quadratic surfaces. In closing this section we note that Shepard's formula can also be inter reted as arising from weighted least squares--see section 5.1.

3.4 Spline interpolation (scattered data). Suppose X is a linear space of "smooth" functions defined on the domain D, and let

(3.18) $U = \{f \in X: f(x_i,y_i) = F_i, \ i = 1,2,\ldots,N\}$.

U is the set of smooth functions which interpolate. Now suppose that θ is a functional on X which measures the smoothness of an element in X--the smaller $\theta(f)$ is, the smoother f is. Then we may consider the following minimization problem:

(3.19) Find $s \in U$ such that $\theta(s) = \inf_{u \in U} \theta(u)$.

The function s will be the smoothest interpolant, and in view of the similarity with classical spline approximation, s is called a spline function interpolating F. The basic questions concerning spline interpolation center around existence, uniqueness, characterization, and construction. A quite general

abstract theory of spline interpolation has been built up (see eg. Laurent [127] and references therein). In this section we quote some specific examples which can be used on Problem 1.1.

Where X is a semi-Hilbert space, $\theta(f) = \|f\|$, where $\|\cdot\|$ is a seminorm on X, and $N = \{f \in X: \|f\| = 0\}$, it is possible to show (under some additional mild conditions on X, see Duchon [72,73]) that problem (3.19) always has a solution which is unique up to an element in N. Moreover, it can be shown that there exists a reproducing kernel K defined on $D \times D$ such that

$$(3.20)\quad s(x,y) = \sum_{i=1}^{N} a_i K((x,y);(x_i,y_i)) + \sum_{i=1}^{d} b_i p_i(x,y),$$

where $\{p_i\}_1^d$ is a basis for N. Moreover, the coefficients $\{a_i\}$ and $\{b_i\}$ can be determined from the linear system of equations

$$(3.21)\quad \sum_{j=1}^{N} K((x_j,y_j);(x_i,y_i))a_i + \sum_{i=1}^{d} b_i p_i(x_j,y_j) = F_j, \quad j=1,\ldots,N$$

$$\sum_{i=1}^{N} a_i p_k(x_i,y_i) = 0, \quad k = 1,2,\ldots,d.$$

The development with semi-Hilbert spaces in Duchon [72,73] is an extension of earlier work of Atteia [10-12] and Thomann [192-193] using Hilbert spaces. The essential difficulty in applying the general results is the construction of an appropriate reproducing kernel. We turn now to some specific examples.

Suppose X is the space of all functions on the rectangle $D = H$ (cf. (3.4)) which have (distributional) derivatives up to order 2 which lie in $L^2(H)$. For $f \in X$, let

$$(3.22)\quad \theta(f) = \iint_D |D_x^2 f|^2 + 2|D_x D_y f|^2 + |D_y^2 f|^2.$$

The reproducing kernel in this case can be written down as an infinite series involving sin and cos, and the space N is spanned by 1, x, and y. Similarly, if we replace H by the unit disc UD, the kernel can be computed as an infinite series (see Atteia [10-12] and Thomann [192-193]). Thomann considers computation of these splines by approximating the infinite series--FORTRAN programs are also included.

If we replace the bounded sets H or UD by the entire plane R^2 and introduce an appropriate space X, it is possible to obtain explicit expressions for the reproducing kernel. This is the content of Duchon [72,73]. In particular, let $\tilde{H}^s$ be the set of all tempered distributions f on R^2 whose Fourier transforms $\hat{f}$ satisfy $\int |\hat{f}| t^{2s} dt < \infty$. Let X^{ms} denote the set of all functions which have derivatives up to order m lying in $\tilde{H}^s$. Our first example concerns the space X^{20}. If we choose Θ as in (3.22), then the interpolating spline solution of (3.19) is of the form

$$(3.23) \quad s(x,y) = \sum_{i=1}^{N} a_i r_i^2(x,y) \log (r_i(x,y)) + b_1 x + b_2 y + b_3,$$

where $r_i(x,y) = [(x-x_i)^2 + (y-y_i)^2]^{\frac{1}{2}}$. The coefficients are determined from the system (3.21) with $d = 3$, $N = \text{span}\{1,x,y\}$, and $K(z,w) = |z-w|^2 \log(z-w|$. Duchon refers to this type of spline as a thin plate spline since the expression Θ relates to the energy in a thin plate forced to interpolate the data. This spline belongs to $C(R^2)$.

As a second example, suppose we consider $X = X^{21}$. In this case the solution of (3.19) with Θ given by (3.22) has the form

$$(3.24) \quad s(x,y) = \sum_{i=1}^{N} a_i (r_i(x,y))^3 + b_1 x + b_2 y + b_3.$$

Here $K(z,w) = |z-w|^3$. Duchon [72,73] refers to these splines

as pseudo-cubic splines because of the analogy with the cubic splines in one variable. They belong to $C^1(R)$. Pseudo quintic splines etc. are also considered in Duchon [72, 73].

A similar program has been carried out by Mansfield [133-137] for some spaces of smooth functions defined on a rectangle H. In [136] she considers a space of functions $T^{m,n}(\alpha,\beta)$, where m and n are positive integers and $a \le \alpha \le b$, $c \le \beta \le d$. This space is actually defined by completion of a set of tensor product functions with respect to an appropriate inner-product, and we do not want to define it precisely here. A function $f \in T^{m,n}(\alpha,\beta)$ has the following properties, however:

$$(3.25)\quad \begin{cases} f^{(i,j)} \in C(H), \quad i = 0,1,\ldots,m-1 \text{ and } j = 0,1,\ldots,n-1 \\ f^{(s-j-1,j)}(x,\beta) \in AC[a,b] \text{ and } f^{(s-j,j)}(x,\beta) \in L^2[a,b], \\ \qquad\qquad j = 0,1,\ldots,n-1 \\ f^{(i,s-i-1)}(\alpha,y) \in AC[c,d] \text{ and } f^{(i,s-i)}(\alpha,y) \in L^2[c,d], \\ \qquad\qquad i = 0,1,\ldots,m-1 \\ f^{(m-1,n-1)} \in AC(H) \text{ and } f^{(m,n)} \in L^2(H), \end{cases}$$

where AC stands for the space of absolutely continuous functions and where $s = m + n$. By constructing an appropriate reproducing kernel, she is able to solve problem (3.19) with

$$(3.26)\quad \theta(f) \quad \iint_H [f^{(m,n)}]^2 + \sum_{j=0}^{n-1} \int_a^b [f^{(s-j,j)}(x,\beta)]^2 dx + \sum_{i=0}^{m-1} \int_c^d [f^{(i,s-i)}(\alpha,y)]^2 dy.$$

In [133], Mansfield carries out a similar analysis for a space of functions $R^{m,n}$ defined on the rectangle H. Here $R^{m,n} \subset L_2^m[a,b] \times L_2^n[c,d]$, where $L_2^m[a,b]$ is the usual Sobolev space of functions with absolutely continuous derivatives up to order m-1, and with $f^{(m)} \in L^2[a,b]$. By constructing an

appropriate reproducing kernel, she now solves problem (3.19) with

$$(3.27)\quad \theta(f) = \iint_H [f^{(m,n)}]^2 + \sum_{j=0}^{n-1} \int_a^b [f^{(m,j)}(x,c)]^2 dx + \sum_{i=0}^{m-1} \int_c^d [f^{(i,n)}(a,y)]^2 dy .$$

The solution turns out to be a piecewise polynomial of degree $2m-1$ in x and of degree $2n-1$ in y. It is also in $C^{2m-2,2n-2}(H)$. For the particular case of gridded data, it reduces to the tensor product of one-variable splines (cf. the following section). Other more general definitions of θ are also considered (with minor modifications on the one-dimensional integrals).

A more algebraic approach to constructing multidimensional spline functions (which also involves certain kernel functions) has been taken by Schaback [173-174]. His two-dimensional kernel function is obtained as a tensor product of one-dimensional kernels.

3.5. Spline interpolation (gridded data). The problem of constructing interpolating splines in two dimensions with gridded data as in (3.4)-(3.6) is, of course, a special case of the general problems discussed in subsection 3.4. The development of the gridded data case predated the more general development and, moreover, is considerably simpler. There are a great many papers on two-dimensional polynomial splines and generalizations. We do not have space here to discuss all of them in detail. We shall be content to quote some of the papers and to give a somewhat more complete discussion of polynomial splines, which are the most widely used splines for this problem.

Some early papers dealing with two-dimensional interpolating splines include Birkhoff and de Boor [26], Birkhoff and

Garabedian [27], Price and Simonson [159], and Theilheimer and Starkweather [191]. In [26] certain bicubic splines were introduced which were later studied in detail in de Boor [32]. The problem was to minimize

$$(3.28)\quad \int_a^b \int_c^d [f^{(2,2)}(x,y)]^2 dxdy$$

over all appropriately smooth functions on the rectangle H which interpolate the gridded data (3.4)-(3.6). It was found that the solution of this problem was a certain bicubic function with global smoothness $C^2(H)$. This problem was generalized to minimizing

$$(3.29)\quad \theta(f) = \int_a^b \int_c^d [f^{(m,n)}(x,y)]^2 dx\, dy, \quad m = 2p,\ n = 2q$$

in Ahlberg, Nilson and Walsh [1,2], whose solution involves certain higher-order polynomial splines. Since they are widely used, we give a short algebraic treatment here.

The points $\{x_i\}_0^{k+1}$ and $\{y_j\}_0^{\ell+1}$ define a partition of the intervals $[a,b]$ and $[c,d]$, respectively (cf. (3.5)). Suppose now that $x_{1-m} \le \dots \le x_{-1} \le a < b \le x_{k+2} \le \dots \le x_{k+m-1}$ and $y_{1-n} \le \dots \le y_{-1} \le c < d \le y_{\ell+2} \le \dots \le y_{\ell+n-1}$ are chosen arbitrarily. Let $\{N_i^m\}_{1-m}^k$ be the B-splines associated with the x-partition, and let the B-splines associated with the y-partition be denoted by $\{N_j^n(y)\}_{1-n}^{\ell}$. For a complete discussion of B-splines and their properties, see de Boor [36] in this volume (or [33]). Let

$$(3.30)\quad N_{ij}(x,y) = N_i^m(x) N_j^n(y), \quad i = 1-m,\dots,k \text{ and } j = 1-n,\dots,\ell.$$

The linear space

$$(3.31)\quad \mathcal{S} = \text{span}\,\{N_{ij}(x,y)\}_{i=1-m,\,j=1-n}^{k,\,\ell}$$

is clearly of dimension $(k+m)(\ell+n)$. We may now construct an

element in (3.31) which interpolates to the gridded data.

Since there are only $(k+2)(\ell+2)$ data points on the grid (cf. (3.4)-(3.6), it is clear that if we use s to interpolate, we have

$$(3.32)\quad (k+m)(\ell+n)-(k+2)(\ell+2) = (k+2)(n-2)+(\ell+2)(m-2)+(n-2)(m-2)$$

free parameters. Thus, to uniquely define a spline, one must add additional conditions. Recall that $m = 2p$ and $n = 2q$. Then we might add the extra conditions

$$(3.33)\quad \begin{aligned} s^{(\nu,0)}(x_0,y_j) &= s^{(\nu,0)}(x_{k+1},y_j) = 0, \quad \begin{matrix} j=0,1,\ldots,\ell+1 \\ \nu=p,\ldots,m-2 \end{matrix} \\ s^{(0,\mu)}(x_i,y_0) &= s^{(0,\mu)}(x_i,y_{\ell+1}) = 0, \quad \begin{matrix} i=0,1,\ldots,k+1 \\ \mu=q,\ldots,n-2 \end{matrix} \end{aligned}$$

and

$$(3.34)\quad \begin{aligned} s^{(\nu,\mu)}(x_0,y_0) &= s^{(\nu,\mu)}(x_0,y_{\ell+1}) = s^{(\nu,\mu)}(x_{k+1},y_0) \\ &= s^{(\nu,\mu)}(x_{k+1},y_{\ell+1}) = 0, \quad \begin{matrix} \nu=p,\ldots,m-1 \\ \mu=q,\ldots,n-1. \end{matrix} \end{aligned}$$

These are called the natural boundary conditions, and it can be shown that the system of equations

$$(3.35)\quad \sum_{i=1-m}^{k}\sum_{j=1-n}^{\ell} a_{ij}N_{ij}(x_\alpha,y_\beta) = F_{\alpha\beta}, \quad \begin{matrix} \alpha=0,1,\ldots,k+1 \\ \beta=0,1,\ldots,\ell+1 \end{matrix}$$

coupled with the conditions (3.33)-(3.34) provides a nonsingular system of equations for the coefficients $\{a_{ij}\}$. This system has convenient bandedness properties if the equations are arranged properly. The resulting spline is precisely the solution of the minimization problem (3.29). The boundary conditions (3.33)-(3.34) are the natural ones associated with the problem (3.29). However, it is also possible to specify lower-order derivative information along the boundary and also obtain a nonsingular system of equations. The resulting spline, called Type I, can also be shown to satisfy an appropriate minimization

problem. However, for data-fitting purposes, to use the interpolant with boundary derivative data one would first have to perform a first-stage approximation to find estimates for the required derivatives.

The best-known case of the above spline interpolation is the case $m = n = 4$, i.e., bicubic spline interpolation. In this case the surface constructed is a piecewise bicubic with global smoothness $C^2(H)$. The natural boundary conditions set second-derivative values to 0. Programs for computing natural bicubic interpolating splines can be found in the IMSL Library [117] in FORTRAN. FORTRAN programs for Type I bicubic splines can be found in Koelling and Whitten [121], where the required boundary information is assumed to be input. An ALGOL program for computing Type I bicubic splines in which boundary data are automatically computed by fitting one-dimensional splines appears in Späth [183].

Bicubic spline interpolation has been widely applied. For some references in the Geology literature, see eg. Anderson [7], Bhattacharyya [22], Holroyd and Bhattacharyya [115], Koelling and Whitten [121], and Whitten and Koelling [206].

Problem (3.29) has been widely generalized in the spline literature. Instead of minimizing ordinary derivatives, one may introduce general linear operators, and instead of dealing with point evaluation functionals, more general linear functionals may be permitted. To list some (but by no means all) papers dealing with such generalizations, we mention Arthur [8,9], Birkhoff, Schultz and Varga [29], de Boor [34], Delvos [65,66], Delvos and Schempp [68,69], Delvos and Schlosser [70], Fisher and Jerome [78,79], Haussmann [100], Haussmann and Munch [104], Munteanu [143,144], Nielson [148,150], Ritter [164,165], Sard [171,172], Schoenberg [176], Schultz [177,178], Späth [184,185], and Zavialov [209-212]. On L-shaped regions and other polygons

see Birkhoff [25] and Carlson and Hall [44-49].

We close this section by mentioning another direction of generalization which has led to a considerable development, the idea of spline blending. These methods are useful for construction of a surface which interpolates not only function values at isolated points but on the grid lines themselves; i.e.,

$$(3.36)\quad f(x,y_j) = F(x,y_j) \qquad a \le x \le b \quad \text{and} \quad j = 0,1,\ldots,\ell+1$$
$$f(x_i,y) = F(x_i,y) \qquad c \le y \le d \quad \text{and} \quad i = 0,1,\ldots,k+1.$$

To use such blending methods one must have F defined on the grid lines. Thus, the methods could be of value as second-stage processes. We do not have space to go into detail on spline-blended methods. We refer to the recent book of Barnhill and Riesenfeld [20] for a collection of papers on the subject and for further references. See also the papers of Gordon [84-87] and Gordon and Hall [88]. Recently, considerable effort has gone into showing that blending methods also arise as solutions of appropriate variational problems; see the papers of Delvos [65], Delvos and Kosters [66], and Delvos and Malinka [67].

4. Local interpolation methods

The interpolation methods discussed in section 3 were global in nature--that is, the value $f(x,y)$ of the constructed surface at any given point (x,y) in D depends on the values of all of the data points. This generally means that to compute a representation for f one has to solve a fairly large system of equations, and to evaluate $f(x,y)$ one generally has to carry out a considerable amount of arithmetic. In this section we shall consider local schemes where the surface depends only on nearby data points. Then the construction will usually lead to (a possibly large number) of <u>small</u> systems of equations, and moreover, the evaluation of the surface at a given point will

usually involve very little computation.

Many of the schemes mentioned in section 3 can be made local in nature by the following simple approach. Suppose that the domain D is partitioned into subdomains: $D = \bigcup_{i=1}^{d} D_i$. We then seek a surface in the form

$$(4.1)\quad f(x,y) = \{f_i(x,y), \quad (x,y) \in D_i, \quad i = 1,2,\ldots,d.$$

To construct each individual f_i, we suppose that $\tilde{D}_i$ are domains containing D_i, which contain only points which are "near" D_i. Then we use the data (and only the data) in $\tilde{D}_i$ to construct f_i. Usually, we can choose $\tilde{D}_i = D_i$. In most cases the most convenient choices for the subdomains D_i are triangles and rectangles. We discuss these two cases first.

4.1. Triangular subregions (scattered data). Suppose that we are given data at points $P_i = (x_i,y_i)$, $i = 1,2,\ldots,N$ scattered throughout the plane, and let D be the convex hull of these points. It is more or less clear that by drawing lines from point to point we can construct a set of triangles with vertices at the P_i which partition D. It is also clear that given any set of points, this triangularization of D is not usually uniquely defined (see Figure 2 below for two different triangularizations of the same region). Moreover, as the figure shows, some triangularizations are superior to others in the sense that they exhibit fewer of the less desirable long thin triangles.

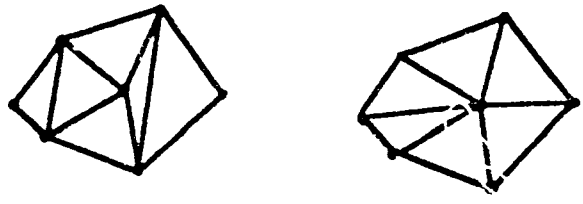

Figure 2. Triangularization

The design of an algorithm to divide a region into acceptable triangles with vertices at prescribed points is not as easy as it sounds. Two algorithms in the literature which are designed to give good triangularizations can be found in Cavendish [50] and in Lawson [128].

The simplest approach to defining a local interpolating surface is to construct $f_i(x,y)$ to be of the form $a_1 + a_2x + a_3y$ in each triangle. The data at the three corners of the triangle determine the coefficients for that piece of f (the corresponding system will be nonsingular provided the triangle is nondegenerate). This procedure produces a piecewise linear surface which, in fact, will be globally continuous. This last property follows from the fact that along the sides of the triangle the functions reduce to straight lines joining the vertices. This method has been used by several authors for data fitting, e.g., Lawson [128] and Whitten [206]. For some contouring routines based on this local interpolation scheme, see section 8.

If we desire to interpolate several sets of data defined on the same triangularization, it may be more convenient to compute Lagrangian functions rather than to compute the surface in each triangle separately. In particular, it is clear that we can construct functions $\{\phi_j(x,y)\}_1^N$ with the property

$$\phi_j(x_i,y_i) = \delta_{ij}, \quad i,j = 1,2,\ldots,N. \tag{4.2}$$

These functions can be constructed as pyramids in such a way that the function ϕ_j has support only on the triangles surrounding the point (x_j,y_j) (see Figure 3). In terms of these Lagrangian functions, the interpolating surface is given by

$$f(x,y) = \sum_{j=1}^{N} F_j\phi_j(x,y). \tag{4.3}$$

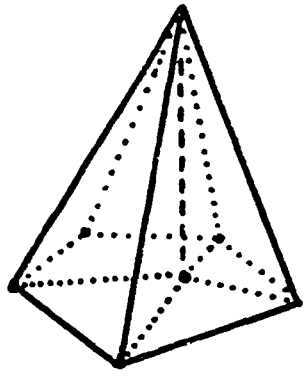

Figure 3. A Lagrange Element

The Lagrangian approach to local interpolation is very reminiscent of the finite element method in which the solution of an operator equation is sought in the form of a linear combination of a set of functions (called elements) with the property (4.2). (See e.g., Prenter [157], Schultz [179], or Strang and Fix [188].) There is no need to restrict the elements to be piecewise linear functions--we may use higher-order polynomials, rational functions, or even more complicated functions. In fact, if we are careful in the construction, we may be able to construct elements with small support but higher global smoothness.

There are a great many papers in the finite-element literature concerned with defining convenient smooth elements (Lagrangian functions with small support). To mention a few, see Barnhill, Birkhoff, and Gordon [16], Barnhill and Gregory [17, 18], Barnhill and Mansfield [19], Birkhoff and Mansfield [28], Bramble and Zlamal [39], Goel [83], Hall [94], Mitchell [141], Mitchell and Phillips [142], Nicolaidis [146,147], Zenisek [213], Zienkowicz [214], and Zlamal [215-217]. The books on finite elements of Aziz [13], de Boor [35], Strang and Fix [188], and Whiteman [198] should also be consulted.

The construction of elements with higher-order smoothness becomes increasingly difficult. For example, it is shown in Mansfield [137] that to get an element with support on the triangles surrounding P_j and with global continuity $C^1(D)$, it is necessary to use polynomials of degree 5 at least. (Matters are somewhat simpler on regular triangularizations, see subsection 4.2 below.)

We close this subsection by mentioning that it is also possible to perform interpolation using elements based on triangles to data which also involves derivatives, or in analogy with the blending methods, to data which includes function values along the edges of the triangles. (See e.g., Barnhill, Birkhoff, and Gordon [16], or Barnhill and Gregory [17,18].) These methods are not directly applicable to the scattered data Problem 1.1, but may be useful as second-stage methods.

4.2. Regular triangularizations. When the data is distributed such that the region can be triangulated into a set of congruent triangles, then it is extremely advantageous to use the Lagrange approach. In particular, in this case we can find an element ϕ with value 1 at (0,0) such that all other elements are translates of ϕ. In this case, f takes the form

$$(4.4)\quad f(x,y) = \sum_{j=1}^{N} F_j \phi((x,y) - (x_j,y_j)).$$

We illustrate this with a couple of examples. Suppose that we are given data at points chosen from the collection

$$(4.5)\quad \Omega_1 = \{(i,j)\}_{i,j\in Z} \cup \{(i+\tfrac{1}{2}, j+\tfrac{1}{2})\}_{i,j\in Z}, \quad Z = \{\text{integers}\}.$$

These points lie on the corners of a triangular grid as shown in Figure 4.

It is shown in Zwart [218,p.673] that there exists a function $\phi \in C^1(R^2)$ which is 1 at the origin and 0 at all other points in Ω, and has support on the shaded region in Figure 4.

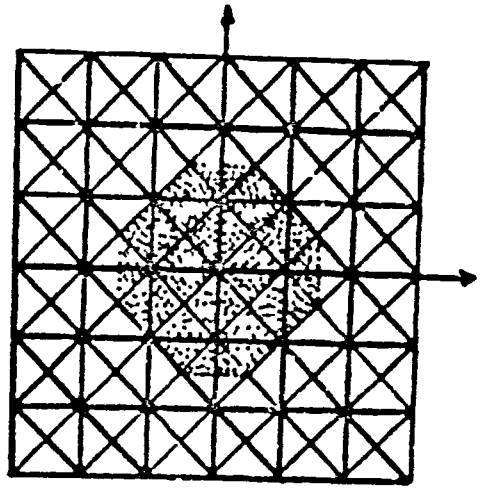

Figure 4. A Regular Triangularization

This function is constructed as a piecewise quadratic polynomi A similar element has been constructed by Powell [156] (th ure on page 267 of [156] should be rotated 45° to see t' .

To give another example, suppose that we consider the set of points Ω_2 which lie at the vertices of the grid defined by equilateral triangles shown in Figure 5.

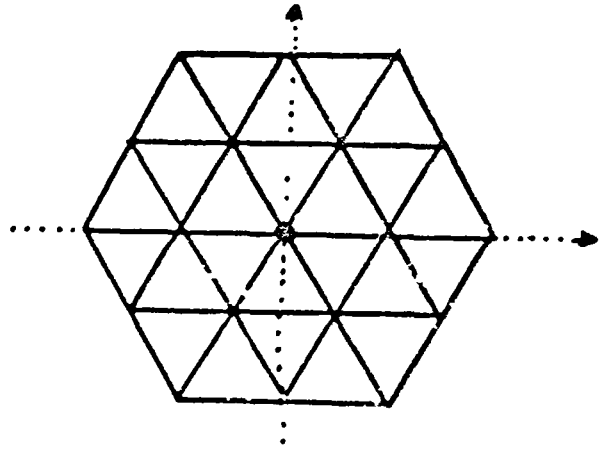

Figure 5. Another Regular Triangularization

It is shown in Fredrickson [81] that there exists a function ϕ which has value 1 at the origin and value 0 at all other points in Ω_2. The function ϕ is in $C^2(R^2)$, consists of piecewise quartics, and has support in the region shown in Figure 5. Fredrickson also constructs a piecewise cubic element with the same support but which is only $C^1(R^2)$. For right triangles see Carlson and Hall [44].

4.3. Rectangular subregions. In this section we suppose that we have data given at points lying on a rectangular grid as in (3.4)-(3.6), and consider local interpolation methods. The simplest approach here (cf. the triangularization case) is to construct a separate bilinear function $f(x,y) = a_1 + a_2x + a_3y + a_4xy$ in each subrectangle, $H_{ij} = [x_i,x_{i+1}] \times [y_j,y_{j+1}]$, using the four corner values to determine the coefficients. Since the bilinear patches reduce to linear functions on the grid lines, the global surface is $C(R)$.

Several authors have considered constructing functions on each of the H_{ij} using higher-order polynomials. This requires additional information in addition to the four corner values. For example, if one seeks a bicubic

$$(4.6) \quad f(x,y) = \sum_{i=0}^{3} \sum_{j=0}^{3} a_{ij} x^i y^j,$$

there are 16 coefficients to determine. These could be determined by the four corner values, plus the values of f_x, f_y, and f_{xy} at each corner. To determine these, one must perform some first-stage process. For some approaches to this, see Akima [5], Hessing, et al [114], and Shu, et al [181]. A FORTRAN program for Akima's method can be found in [6]. Nonpolynomial patches have also been considered; e.g., see Birkhoff and Garabedian [27].

The Lagrange (finite element) approach can also be used in

the case of rectangular gridded data. In particular, if we can construct a function satisfying (4.2) with local support, then the surface f given by (4.3) will interpolate and the method will be local in character. As before, the Lagrange approach is especially convenient if the grid is regular, i.e., if all subrectangles H_{ij} are congruent. To illustrate this, suppose that the H_{ij} are actually the unit squares; i.e., the data points lie in the set

(4.7) $\Omega_3 = \{(i,j)\}$ $i,j \in Z$, $Z = \{\text{integers}\}$.

To get a quadratic C^1 element, we may simply rotate the element of Zwart [218] considered in the last section by 45 degrees (cf. Figure 4), or we may take the element of Powell [156].

4.4. Parametric representations. The methods discussed in the last section is concerned with data given on a rectangular grid. By using parametric representations, it is possible to construct similar local interpolating surfaces for data given at the corners of any partition of D consisting of quadrilaterals. In this section we briefly describe how this might proceed.

Suppose Q is a particular quadrilateral subregion of D of interest. In addition, suppose that $x(s,t)$, $y(s,t)$, and $z(s,t)$ are functions defined on the unit square $U = [0,1] \times [0,1]$ with the properties that as (s,t) runs over the boundary of U, $(x(s,t),y(s,t))$ runs over the boundary of the quadrilateral; the four corners of U correspond to the four corners of Q; and $z(s,t)$ takes on the desired data values at the four corners of U. In this case, the triple $(x(s,t),y(s,t),z(s,t))$ provides a parametric representation of a piece of surface defined over Q interpolating the data.

The problem of constructing parametric representations of interpolating functions has been considered in a number of papers. Several papers on these methods and a host of references can be found in the book of Barnhill and Riesenfeld [20]; see

also the survey paper of Shu et al [181]. Such surfaces are sometimes called Coon's surfaces, cf. Coons [59], and are of considerable interest in the field of computer-aided geometric design. To mention just a few of the actual papers, see Ahuja and Coons [4], Earnshaw and Youille [74], Ferguson [77], Hayes [107], Hosaka [116], and Mangeron [132].

There also has been some effort directed towards constructing elements (Lagrange functions) associated with other less regular subsets of the plane We mention, for example, the work of Ciarlet and Raviart [55], Wachspress [194,195], and Zlamal [217] in which elements are constructed for domains involving curved edges.

4.5. Local Shepard methods. It is possible to modify the method discussed in subsection 3.3 to make it local. For example, following Shepard [180], suppose we fix $0 < R$ and define

$$(4.8)\quad \psi(r) = \begin{cases} 1/r & 0 < r \le \frac{R}{3}, \\ \frac{27}{4R}\left(\frac{r}{R} - 1\right)^2, & R/3 < r \le R, \\ 0 \quad , & R < r \quad . \end{cases}$$

This function is continuously differentiable and vanishes identically for $r < R$. Now with r_i as in (3.8), we define

$$(4.9)\quad f(x,y) = \begin{cases} \dfrac{\sum_{i=1}^{N} F_i [\psi(r_i)]^{\mu}}{\sum_{i=1}^{N} [\psi(r_i)]^{\mu}}, & \text{when } r_i \neq 0, \text{ all } i \\ F_i \quad , & \text{when } r_i = 0. \end{cases}$$

Formula (4.9) is defined at all (x,y) in the plane R^2. By definition it interpolates the values F_i at the data points (x_i,y_i), $i = 1,2,\ldots,N$. The values at non-data points are obtained as weighted averages of the data values F_i, but

only those which lie at points within a distance of R of (x,y). Thus, the formula is local.

To use this method in practice it is necessary to choose a reasonable value for R. The aim is to find R so that for every (x,y) a reasonable number of data points will fall in the disk centered at (x,y) of radius R. It would also be possible to let R depend on (x,y), i.e., to use different values of R in different subregions of D.

5. Global approximation

As mentioned in the introduction, frequently the data does not warrant constructing an interpolating function (e.g., because of errors). In such cases it may be preferable to construct a surface which only approximates the data. In this section we discuss some global approximation methods.

5.1. Polynomial least squares. The general theory of discrete least-squares fitting is very well known. To briefly review, suppose that $\{\phi_j\}_1^n$ are n given functions on D. Define

$$(5.1)\quad \Phi(a) = \sum_{i=1}^{N} \left| \sum_{j=1}^{n} a_j \phi_j(x_i,y_i) - F_i \right|^2,$$

where $a = (a_1,\ldots,a_n)^T$ is any vector in R^n. Then the problem is to find a^* such that

$$(5.2)\quad \Phi(a^*) = \min_a \Phi(a).$$

The corresponding function

$$(5.3)\quad f(x,y) = \sum_{j=1}^{n} a_j^* \phi_j(x,y)$$

is called the discrete least-squares approximation of the data $\{F_i\}_1^N$. Usually one takes n considerably smaller than N. In this section we briefly discuss least squares using polynomials. Before doing so, however, we make a few general remarks about

solving the general least-squares problem.

There are several approaches to solving (5.2). Perhaps the neatest is the case where the $\{\phi_j\}_1^n$ are orthonormal with respect to the inner-product

$$(5.4) \quad (\phi,\psi) = \sum_{i=1}^{N} \phi(x_i,y_i)\psi(x_i,y_i).$$

Then the solution of (5.2) can be written down explicitly as

$$(5.5) \quad f(x,y) = \sum_{j=1}^{n} a_j^* \phi_j(x,y).$$

A second very well-known approach to solving (5.2) is via the normal equations

$$(5.6) \quad A^*A\,a = A^*F,$$

where $F = (F_1,\ldots,F_N)^T$ is the vector of data values, and where

$$(5.7) \quad A = (\phi_j(x_i,y_i))_{j=1,i=1}^{n,N}.$$

In some cases the normal equations are a perfectly acceptable way to compute least-squares approximation, but in other cases the system (5.6) may be ill-conditioned (or even singular--cf. the following subsection for spline least squares). This approach is also not convenient should side conditions be desired (e.g., by imposing actual interpolation at some of the values). For more on the normal equations, see any book on Numerical Analysis.

A more modern method of solving least-squares problems is to use general matrix methods. Specifically, consider the observation equations

$$(5.8) \quad A\,a = F.$$

It can be shown that by applying a series of matrix transformations to this system, one can obtain a set of equations giving the vector a^*. For a complete description of methods of this

type see Lawson and Hanson [129] or Stewart [187]. Matrix methods are quite amenable to the adding of side conditions and can also be designed to take account of rank-deficiency of the matrix A (which corresponds to the case of singular normal equations).

Polynomial discrete least-squares fitting has been widely used for fitting surfaces to data, both scattered and regular. Several authors have developed algorithms for polynomial discrete least-squares fitting of scattered data by constructing orthonormal polynomials (e.g. by Gram-Schmidt orthonormalization). See, for example, Cadwell and Williams [42], Crain and Bhattacharyya [61], and Whitten [201,202]. The latter contains a FORTRAN program.

When the data are more regularly distributed, polynomial least-squares fitting can often be simplified. For example, if the data lie on a grid as in (3.4)-(3.6), then the desired orthogonal polynomials are simply products of the one-dimensional orthogonal polynomials associated with the one-dimensional inner products corresponding to $\{x_i\}_0^{k+1}$ and $\{y_j\}_0^{\ell+1}$ respectively; e.g., see Cadwell [41] or Clenshaw and Hayes [56], as well as the survey papers of Hayes [105,108,109].

There are also special methods for handling data which are not on a grid but instead lie on parallel straight lines. For example, Clenshaw and Hayes [56] have developed methods using expansions in terms of Tchebycheff polynomials (although the method actually only produces an approximation to the least-squares fit rather than the actual minimum).

Polynomial least squares can also be interpreted as multidimensional regression as practiced by statisticians, e.g., see Efroymson [75]. For example, if we are trying to fit a function in the form

$$f(x,y) = \sum_{i=0}^{dx} \sum_{j=0}^{dy} a_{ij} x^i y^j,$$

then by defining new variables by

$$z_{\nu(dy+1)+\mu} = x^\nu y^\mu, \qquad \begin{matrix} \nu = 0,1,\ldots,dx \\ \mu = 0,1,\ldots,dy \end{matrix}$$

we can write

$$f(x,y) = \sum_{i=0}^{d} b_i z_i, \qquad d = dxdy + dx + dy,$$

and the problem becomes one of fitting a <u>linear</u> function in several variables.

We close this section by observing that in some cases it may be desirable to consider <u>weighted</u> least squares. In particular, if we have positive weights $w_i > 0$, $i = 1,2,\ldots,N$, then we may replace Φ in (5.1) by

$$I_w(a) = \sum_{i=1}^{N} w_i \left| \sum_{j=1}^{n} a_j \phi_j(x_i,y_i) - F_i \right|^2 .$$

It is interesting to note that the interpolation formula of Shepard discussed in section 3.3 can be interpreted in terms of weighted least-squares fitting. In particular, fix (x,y) in D, and let $r_i(x,y)$ be the distance from (x,y) to the point (x_i,y_i) as before. Now set $w_i = r_i^{-\mu}$, and consider least-squares approximation by a constant c, using these weights. Then one easily computes that the least-squares choice of c is

$$c = \frac{\sum_1^N w_i F_i}{\sum_1^N w_i} = \frac{\sum_1^N F_i r_i^{-\mu}}{\sum_1^N r_i^{-\mu}} .$$

This approach was adopted by Pelto, Elkins and Boyd [152] (as pointed out to me by Chuck Duris).

5.2. Discrete least-squares fitting by splines. As outlined in the previous subsection, discrete least squares can be carried out with any finite set of functions. It is not surprising that a number of authors have tried using tensor product splines. See, e.g., Halliday, Wall, and Joyner [96], Hayes and Halliday [110], Jordan [119], Hanson, Radbill, and Lawson [97], and Whiten [199]. Hayes and Halliday have developed both ALGOL and FORTRAN programs. It is, on the other hand, perhaps somewhat surprising that least-squares fitting with splines can be somewhat problematical. We briefly discuss the method.

Suppose that $H = [a,b] \times [c,d]$ is a rectangle containing the domain D of interest. Let $\{x_i\}_0^{k+1}$ and $\{y_j\}_0^{\ell+1}$ be partitions of $[a,b]$ and $[c,d]$, respectively, and let $\{N_{ij}\}_{1-m,1-n}^{k+1\ \ell+1}$ be the tensor product B-splines discussed in section 3.5. We consider discrete least-squares fitting using these $(k+m)(\ell+n)$ B-splines.

To explain how difficulties can arise with spline least-square fitting, we observe that it is quite easy for the matrix A in the observational equations (5.8) to be rank-deficient. On a trivial level this can happen if for some B-spline N_{ij}, none of the data points lies in its support. This deficiency can, of course, be easily removed by dropping this particular B-spline from the set being used to approximate. But rank deficiency can also occur in more subtle ways because of the local support properties of the functions. This problem can be overcome with properly designed algorithms. See Hayes and Halliday [110] for a careful discussion of spline least-squares fitting. Lawson and Hanson [129] include a general discussion of how to handle rank deficient least-squares problems.

If we operate in terms of the normal equations, then it may well occur that the normal equations are in fact singular. This is again due to the local property of the B-splines com-

bined with the discrete inner-product. Even when it is not singular, the set of normal equations can be ill-conditioned (even though it is a relatively sparse matrix with a kind of repeated band-structure).

Discrete least squares can also be carried out with various finite dimensional linear spaces of blended functions. For an extensive study of such methods, see the dissertation of Doty [71].

5.3. Discrete ℓ_1 and ℓ_∞ approximation. Instead of performing discrete least squares, we may consider the following discrete approximation problem: Given functions $\{\phi_j\}_1^n$ defined on D, we seek a^* so that

$$\Phi(a) = \sum_{i=1}^{N} \left| \sum_{j=1}^{n} a_j \phi_j(x_i, y_i) - F_i \right| \tag{5.9}$$

is minimized. Alternatively, we may minimize

$$\Phi(a) = \max_{1 \le i \le N} \left| \sum_{j=1}^{n} a_j \phi_j(x_i, y_i) - F_i \right|. \tag{5.10}$$

These are the usual ℓ_1 and ℓ_∞ best approximation problems. Both of these problems can easily be reformulated as linear programming problems for the determinations of the optimal a^* (cf. Rabinowicz [160,161] or Rosen [167]). Reasonable choices for the $\{\phi_j\}$ would be low-degree polynomials if D is small, or possibly spline functions.

Discrete approximation methods of this type have had relatively little exposure in the literature. For some results using tensor product splines in the ℓ_∞ problem, see Rosen. The optimal a^* was obtained there by using the standard simplex method on the associated dual linear programming problem.

The ℓ_∞ problem can also be solved by using Remez-type algorithms. For an algorithm which performs generalized

rational approximation (and thus can also be used for polynomial approximations) see Kaufman and Taylor [120]. Theoretical considerations for Tchebycheff approximation in several variables can be found in Collatz [58] or Weinstein [196], for example.

5.4. Spline smoothing (scattered data). In this section we consider some minimization problems similar to those discussed in section 3.4, but where the class of admissible functions is not required to interpolate and where the functional to be minimized includes a term measuring how close the function comes to fitting the data. To be more specific, suppose X is a linear space of "smooth" functions and that θ is a functional on X which measures the smoothness of an element in X. Suppose in addition that E is a functional defined on X which measures how well a function fits the data. Then the spline-smoothing problem is the following:

(5.11) Find $s \in X$ such that $\rho(s) = \inf_{u \in X} \rho(u)$,

where

(5.12) $\rho(f) = \theta(f) + E(f)$.

The abstract theory of spline smoothing has been well developed; see, e.g., the book of Laurent [127] and references therein. To illustrate the ideas, we briefly discuss a couple of examples. We suppose as in section 3.4 that X is a semi-Hilbert space and that θ is a seminorm on X with $N = \{f \in X: \theta(f) = 0\}$. We also suppose that X is actually a function space defined on a domain D, and that the point evaluators at $\{(x_i,y_i)\}_1^N$ are bounded linear functionals on X. We define

(5.13) $E(f) = p \sum_{i=1}^{N} [f(x_i,y_i) - F_i]^2$,

where p is a fixed positive constant. Then it can be shown

(cf. Duchon [72,73]) that the solution of Problem (5.11) is a spline which can be written in the form (3.20), where now the coefficients are determined from the linear system

$$\sum_{i=1}^{N} K((x_j,y_j);(x_i,y_i))a_i + \sum_{i=1}^{d} b_i p_i(x_j,y_j) + a_j/p = F_j,$$

(5.14) $\qquad j = 1,2,\ldots,N,$

$$\sum_{i=1}^{d} a_i p_k(x_i,y_i) = 0, \qquad k = 1,2,\ldots,d.$$

As in section 3.4, the application of this method depends on constructing a reproducing kernel K. If θ is chosen as in (3.22), Atteia [10-12] and Thomann [192,193] considered spline smoothing for spaces of smooth functions on the rectangle and on the disc (the latter even contains ALGOL programs). Duchon [72,73] considers similar problems defined on $D = R^2$.

A similar spline-smoothing problem has also been considered by Pivorarova [154], where θ is taken to be

(5.15) $\qquad \theta(f) = \iint [D_x^2 f]^2 + [D_y^2 f]^2.$

See also Kubik [123].

5.5. Smoothing splines (gridded data). In section 3.5 we considered several minimization problems whose solutions led to interpolating polynomial splines (and generalizations). In conjunction with the development of interpolating splines for gridded data, there was a concurrent development of smoothing splines. For example, instead of minimizing the integral θ in (3.29) over appropriate smooth interpolating functions, we may minimize instead $\rho(f) = \theta(f) + pE(f)$, where E is given by

$$(5.16) \qquad E(f) = \sum_{i=0}^{k+1} \sum_{j=0}^{\ell+1} [f(x_i,y_j) - F_{ij}]^2.$$

For results in this direction, see e.g. Nielson [149,150]. For

θ given by (3.29), the smoothing splines are again polynomial splines. Again, more general linear differential operators and more general linear functionals can be considered.

5.6. Continuous least squares. The method of continuous least squares is not directly suited to fitting surfaces to discrete data, but it can be of use as a second-stage process, so we briefly review it. We suppose now that F is a function defined on D which we wish to approximate, and that $\{\phi_j\}_1^n$ are given functions on D. We define

$$(5.17)\quad \langle f,g\rangle = \iint_D f(x,y)g(x,y)\,dxdy, \quad \|f\|^2 = \langle f,f\rangle$$

and

$$(5.18)\quad \Phi(a) = \|\sum_{j=1}^n a_j\phi_j - F\|^2.$$

The problem is to find a^* to minimize $\Phi(a)$. The solution is given by solving the normal equations

$$(5.19)\quad Aa = r,$$

where

$$A = (\langle\phi_i,\phi_j\rangle)_{i,j=1}^n \quad \text{and} \quad r = [\langle\phi_1,F\rangle,\ldots,\langle\phi_n,F\rangle]^T.$$

For reasonably nice approximating functions it is often possible to compute the normal matrix exactly. In practice, the difficulty lies in evaluating the right-hand sides. Generally a quadrature formula is required for this. One advantage of the method would be that if several data-fitting problems are to be solved using the same set of approximating functions, one can do the work of inverting the normal matrix just once and re-use the result as many times as desired.

Reasonable choices for the approximating functions include polynomials, or better yet, tensor product B-splines as in (3.30). Here the singularity problems do not crop up for the splines because we are integrating instead of summing over

finitely many points. The normal matrix in this case has a kind of repeated band structure. The entries can be computed exactly, e.g., by Gaussian quadrature (cf. de Boor, Lyche and Schumaker [38]). Uniform best approximation by tensor products of splines has also been considered, e.g., see Sommer [182].

6. Local approximation methods

As pointed out at the beginning of section 4, there are many advantages which accrue if one uses local methods rather than global ones. In this section we discuss some local approximation schemes.

6.1. Patch methods. As in the case of interpolation, the simplest approach to obtaining local approximation methods is to partition the domain and to define a surface (patch) on each subdomain separately. In particular, suppose that $D = \cup\{D_i\}_1^d$, where D_i are disjoint subsets of D. Then we may seek f in the form

$$(6.1)\quad f(x,y) = \{f_i(x,y),\ (x,y) \in D_i,\ i = 1,2,\ldots,d.$$

To construct the patch $f_i(x,y)$, we might use the data available in the subregion D_i. In certain cases, however, it may well occur that no data at all are available in the set D_i. In this case we may choose a somewhat larger set $\tilde{D}_i$ of points "near" D_i, and use the data in $\tilde{D}_i$ to construct f_i. For any given method, it should be possible to make the choice of $\tilde{D}_i$ adaptive so that the size of $\tilde{D}_i$ is kept as small as possible consistent with the amount of data desired for the construction of f_i.

The patch method outlined above can be used with any of the approximation methods discussed in section 5. For example, one might choose to use polynomials (of low order), and to do discrete least-squares approximation. Or, one might use ℓ_1 or ℓ_∞ approximation or some other convenient space (e.g. splines)

instead of polynomials. The main point is to keep the size of each individual patch problem (and thus the size of the corresponding system of equations) small. We may have to solve a lot of systems of equations, but each will be small and fairly well-conditioned.

To illustrate how the adaptive feature might be implemented, suppose that the domain D of interest has been enclosed in a rectangle H and that a partition of H is defined by $H = \cup(H_{ij})_{i=0,j=0}^{k,\ell}$, with $H_{ij} = [x_i,x_{i+1}] \times [y_j,y_{j+1}]$ for some

$$(6.2)\quad a = x_0 < x_1 < \ldots < x_{k+1} = b,\ c = y_0 < y_1 < \ldots < y_{\ell+1} = d.$$

Now suppose that we want to do discrete least-squares fitting using a patch of the form $f_{ij}(x,y) = a + bx + cy$ on H_{ij}. In this case it would be reasonable to require that at least 3 pieces of data should be used to construct f_{ij}. If H_{ij} does not contain 3 pieces of data, we expand H_{ij} to $\tilde{H}_{ij}$ by adding all bordering rectangles. If this does not contain 3 pieces, we again add all bordering rectangles, etc. We then compute the discrete least-squares polynomial using the data in $\tilde{H}_{ij}$, but then we use the resulting function only in H_{ij}. The process may be repeated to define each required patch. This kind of adaptive algorithm is very easy to program.

In using patch methods to get local interpolation methods, we concentrated on methods using data at corners of triangles or rectangles, and by choosing appropriate forms for the patches it was possible to get the individual patches to match together to give a continuous global surface (or with more sophisticated patches, even $C^1(D)$ or higher). Here, however, where the individual patches are determined by approximation, it is not very likely that the patches will match up, and the global surface will generally not even be continuous. For most applications, this is a serious drawback. However, as we shall see in

section 7, patch approximation methods can still be very useful as first-stage methods.

6.2. Direct local methods. In this section we discuss some local methods in which the approximating surface is constructed directly from the data without solving any systems of equations. It will be convenient to pose a more general problem than previously considered.

Let $\mathcal{F}$ be a linear space of functions defined on D, and suppose that $\{\lambda_i\}_1^N$ are linear functionals defined on $\mathcal{F}$. Let $\{\phi_i\}_1^N$ be a prescribed set of functions defined on D. Then we are interested in approximation schemes of the following form:

$$(6.3)\quad QF(x,y) = \sum_{i=1}^{N} \lambda_i F \phi_i(x,y).$$

We can think of this as a surface-fitting problem where the data are given by $F_i = \lambda_i F$, $i = 1,2,\ldots,N$. Given the data, we can write the approximation down immediately.

We also observe that if the ϕ_i have support on small subsets of D, and if each λ_i also has support on the same set, then the formula (6.3) is local. For example, if we take λ_i to be point evaluation at the point (x_i,y_i) and $\phi_i(x,y)$ to be a function with support in a neighborhood of (x_i,y_i), then the approximation formula simply becomes

$$(6.4)\quad QF(x,y) = \sum_{i=1}^{N} F_i \phi_i(x,y).$$

This is very reminiscent of the Lagrange form of interpolation (cf. (4.3)), but unless the ϕ_i are taken to satisfy (4.2), QF will not in fact be an interpolant. For this reason, formulae of the form (6.4) (or more generally (6.3)) are sometimes referred to as quasi-interpolants. Local quasi-interpolants of the form (6.3) can be constructed simply by defining the

functions $\{\phi_i\}_1^N$ with local supports. If each of these is continuous (or smooth), then QF will also be.

Although a host of quasi-interpolants can be constructed as outlined above, considerable care must be exercised in order to get methods which give good accuracy (when the original function F is smooth). As observed earlier, this is directly related to making the method exact for polynomials, i.e., such that $QP = P$ for all P in some class of polynomials.

To construct methods of the form (6.3) which apply to scattered data, it is necessary to construct appropriate $\{\phi_i\}_1^N$. While a host of methods can be constructed this way, it is not so easy to choose the ϕ_i to make the method exact for polynomials (which, as we remarked earlier, is directly related to how well the method will approximate smooth functions F). To get methods which do have a reasonable degree of exactness (and a correspondingly good error bound for smooth functions), it is easier to first choose the $\{\phi_i\}_1^N$, and then try to find suitable $\{\lambda_i\}_1^N$. While this generally rules out using point evaluators at scattered data, it is possible to construct methods based on point evaluators at appropriate points, and such methods can be useful as second-stage approximations.

To illustrate these ideas, we consider construction of local spline approximation methods following the general treatment in Lyche and Schumaker [131]. Suppose D is enclosed in a rectangle H, and that H is partitioned into subrectangles by a grid as in (6.2). Suppose that $\{N_{ij}\}_{i=1-m,j=1-n}^{k,\ell}$ are the tensor product B-splines associated with this partition (cf. (3.30)). We are now interested in approximation schemes of the form

$$(6.5)\quad QF(x,y) = \sum_{i=1-m}^{k}\sum_{j=1-n}^{\ell} \lambda_{ij}F N_{ij}(x,y).$$

In particular, we are going to consider the question of

constructing formulae of this type which are exact for the class of polynomials $\mathcal{P}_{v,u}$, with some fixed $1 \le v \le m$ and $1 \le u \le n$. This problem has a very simple algebraic solution if we decide to construct each λ_{ij} in the form

$$(6.6)\quad \lambda_{ij} = \sum_{\nu=1}^{v} \sum_{\mu=1}^{u} \alpha_{ij\nu\mu}\, \lambda^{x}_{ij\nu}\, \lambda^{y}_{ij\mu},$$

where the $\{\lambda^{x}_{ij\nu}\}_{\nu=1}^{v}$ and $\{\lambda^{y}_{ij\mu}\}_{\mu=1}^{u}$ are linear functionals which apply to functions of x and y alone, respectively. It can be shown (cf. [131]) that given any $\{\lambda^{x}_{ij\nu}\}$ and $\{\lambda^{y}_{ij\mu}\}$ satisfying mild independence assumptions, there exist coefficients $\{\alpha_{ij\nu\mu}\}$ such that the formula (6.5) will be exact for $\mathcal{P}_{vu}$. In fact, these coefficients can easily be explicitly computed.

To give one example, suppose

$$(6.7)\quad \begin{cases} \xi_i = \dfrac{(x_{i+1}+\ldots+x_{i+m-1})}{(m-1)}, & i = 1-m,\ldots,k \\ \eta_j = \dfrac{(y_{j+1}+\ldots+y_{j+\ell-1})}{(n-1)}, & j = 1-m,\ldots,\ell. \end{cases}$$

Then we obtain

$$(6.8)\quad QF(x,y) = \sum_{i=1-m}^{k} \sum_{j=1-n}^{\ell} F(\xi_i,\eta_j) N_{ij}(x,y),$$

a formula which exactly reproduces the bilinear polynomials $\mathcal{P}_{1,1}$. This is the multidimensional (tensor product) version of the Variation Diminishing method of Marsden and Schoenberg; it was studied in some detail in Munteanu and Schumaker [145]. This formula is closely related to the Bezier-type surfaces constructed in Riesenfeld [163] (see also Gordon and Riesenfeld [89]).

We should observe that the way formula (6.5) now stands, it may involve information on F which is taken from data outside of the domain D. This situation can be rectified as follows:

Let

(6.9) $\Omega = \{(i,j):$ support $\lambda_{ij} \cap D$ not empty$\}$.

Then it can be shown [131] that the method

$$(6.10)\quad QF(x,y) = \sum\sum_{(i,j)\in\Omega} \lambda_{ij} FN_{ij}(x,y)$$

remains exact as long as all functions are restricted to D.

To get higher-order methods, depending only on point evaluations, we proceed as follows. Choose

$$(6.11)\quad \begin{aligned} x_i &< \tau^x_{ij\nu} < x_{i+m}, \quad \nu = 1,2,\ldots,v \\ y_j &< \tau^y_{ij\mu} < y_{j+n}, \quad \mu = 1,2,\ldots,u, \end{aligned}$$

for $i = 1-m,\ldots,k$ and $j = 1-n,\ldots,\ell$. Then if we take $\lambda^x_{ij\nu}$ to be point evaluation at $\tau^x_{ij\nu}$ and $\lambda^y_{ij\mu}$ to be point evaluation at $\tau^y_{ij\mu}$, the coefficients in (6.6) are easily computed. Hints on where the τ's should be placed within the support of the B-splines are given by the error analysis in [131].

We close this section with some historical remarks on the development of local approximation schemes in two dimensions. Early papers include Babuska [14], de Boor and Fix [37], and Fix and Strang [80]. For some methods involving triangular partitions, see Fredrickson [82]. Quasi-interpolants were constructed in de Boor and Fix [37] using point evaluation data, but including derivatives. We have followed Lyche and Schumaker [131] where general linear functionals are considered, and where in particular, methods can be constructed using only point evaluation of the function. (Local integrals etc. would also be possible.) The papers [37] and [131] both contain extensive error bound analyses. It is striking that these local spline approximation methods give optimal order error bounds for smooth functions.

7. Two-stage processes

Many of the methods we have discussed in this paper are only applicable when the data are regularly spaced (and in fact, many surface-fitting methods require specification of derivative data as well as function values). Such methods cannot be applied directly to the scattered data-fitting Problem 1.1. On the other hand, some of the most convenient local interpolating and local approximating methods which do work for scattered data produce surfaces which are not globally smooth (or even continuous). Thus, it seems natural to consider the possibility of constructing two-stage processes in which the first stage uses the scattered data to construct an approximation g, while the second stage uses g to generate data for constructing a surface f (with desirable properties, such as smoothness).

Since it is quite clear how various methods discussed in the earlier sections might be put together to yield two-stage processes, it will suffice to mention just a couple of examples here.

7.1. Interpolation/interpolation. Suppose that we want to construct a piecewise bicubic surface based on data given on a rectangular grid as in (3.4)-(3.6). In each subrectangle H_{ij} the 16 coefficients of the bicubic f (cf. (4.6)) would be determined by the values of f, f_x, f_y, and f_{xy} at each of the four corners. Now since our original data-fitting problem only specifies the values of the function at the grid points, local interpolation cannot be carried out directly. However, we can use the data to provide estimates for the values of f_x, f_y, and f_{xy} at the grid points (i.e., we construct g interpolating the data); then we can use local bicubic interpolation as a second stage. The reader will have no difficulty in imagining ways to produce estimates for these quantities. For some methods which appear in the literature, see the papers of Akima

[5,6], Koelling and Whitten [121], and Späth [183].

7.2. Approximation/interpolation. Instead of making the first-stage process interpolation as in section 7.1, it would also be possible to use an approximating process. For example, one might use least-squares polynomial approximation to construct a patch surface and then use some convenient interpolation process as a second stage. For an example of this type, see Hessing et al [114].

7.3. Approximation/approximation. This combination is particularly convenient if we are not concerned about getting an interpolating function. Both stages can be made local. To give an example, recently I have constructed an algorithm for fitting surfaces to scattered data in which the first stage consists of polynomial least-squares patch approximation (with adaptive choice of data--see section 6), and where the second stage consists of direct local tensor product spline approximation. Both stages are local, and the final surface is a tensor product spline. Since the second stage is a direct method, it is very cheap to apply. Experiments with real-life data (e.g. from heart potentials, potential fields, and geological maps--see section 2) have produced very promising results. Details, including an analysis of error bounds, will appear elsewhere. I have also tried alternate versions where the patches are constructed as low-order polynomials which are best approximations in the ℓ_1 or ℓ_∞ sense (via linear programming) again with adaptive choice of data. The results were very similar. Finally, I have also experimented with computing patch approximations, followed by continuous least-squares tensor-product spline approximation. Again, the experiments were promising.

8. Contouring

As indicated in the introduction, frequently the goal in

fitting a surface f to data is to construct a contour map which approximates the contour map of the unknown surface F which produced the data. In this section we discuss some methods for constructing contour maps of a surface f.

8.1. Piecewise linear functions on triangles. When the function f to be contoured is a piecewise linear function defined on triangles (and globally continuous), locating contours reduces essentially to a matter of good bookkeeping. Indeed, if H is the height of the contour of interest, then it is easily seen that for a given triangle T with vertices, A, B, and C,

(8.1) the contour does not pass through T if $H < \min(f(A), f(B), f(C))$ or if $H > \max(f(A), f(B), f(C))$

and

(8.2) the contour intersects exactly two sides of T otherwise.

If case (8.2) holds, it is easy to determine which two sides are intersected and, moreover, by using inverse linear interpolation between vertex values, the points on these sides where the contour crosses can be determined. Specifically, if, for example,

$$f(A) < H < f(B),$$

then the contour crosses the line from A to B at the point on the line which is a distance of

$$\frac{(H-f(A))}{(f(B)-f(A))} \, |B - A|$$

from A. Given the points on two sides of a triangle where the contour line crosses, we can now draw the contour line since it is simply a straight line between the points. An algorithm to carry out this procedure requires enumerating the triangles and vertices and some kind of effective search procedure. There are several available in the literature. For ALGOL programs,

see Heap [111,112]. (An earlier paper of Heap and Pink [113] contains a similar FORTRAN program but only for regular triangularizations.) Lawson [128] discusses a similar algorithm. The algorithms mentioned include two possible approaches: (1) one may start with a triangle where it is known the contour intersects, and trace this contour as far as it goes, or (2) one may simply draw the contour lines in all triangles which have them.

8.2. Piecewise bilinear functions on rectangles. Suppose now that the function f to be contoured is a piecewise (continuous) function on a rectangle partitioned into subrectangles by a grid. Since f is linear in x or y on the edges, it follows that we can again determine whether a contour line of height H crosses an edge by inverse linear interpolation. There is in this case, however, a serious difficulty which does not arise in the case of triangles. It may happen that the height H lies on three or even four sides of the rectangle. In this case, it is possible that two different contour lines pass through the rectangle, and it is not clear how to interconnect the points (see Figure 6).

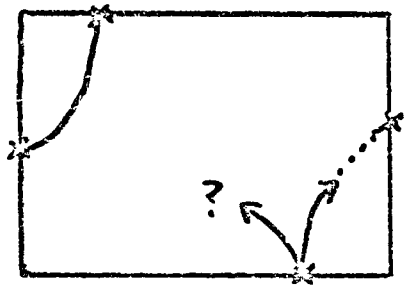

Figure 6. Two Contours in a Rectangle

Put another way, if we are following a contour and enter a rectangle as shown above in Figure 6 on the bottom line, then it is not clear whether we should now turn right or turn left. One approach to designing an algorithm in this case is to simply

always go right, say, even though this may in the end be wrong. (If it is, we have to start over with a coarser mesh.) This technique was incorporated in an algorithm by Heap [111,112]--the paper contains a FORTRAN program. (An earlier ALGOL program can be found in Heap and Pink [113].

A second approach to handling the ambiguity problem is compute an approximation to the value of f at the center of the rectangle (e.g., by taking the average of the four-corner values) and then to triangulate the rectangle. This amounts to a second-stage approximation process, and the surface contoured is no longer f itself but an approximation g. This idea was programmed in ALGOL in Heap and Pink [113] and in FORTRAN in Heap [111,112].

Once the set of points for a particular contour have been found, there are a variety of ways of drawing a contour line through these points. One possibility is to simply draw straight lines between each of the points. The actual contour lines are expressions of the form $y = (a+bx)/(c+dx)$ in each rectangle. These are generally not straight lines. Hence, if smoother contours are desired, one may use any one of a number of methods for drawing a smooth curve through an ordered set of points in the plane. For example, the curve could be computed in parametric form using one-dimensional splines. Another possibility would be to use the Bezier methods with either Bernstein polynomials or with B-splines (cf. Gordon and Riesenfeld [89] and Riesenfeld [163]), although in this case the curves will not exactly go through the points. For other algorithms see Marlow and Powell [138] or McConalogue [139].

8.3. Piecewise quadratics on triangles. Suppose now that f is a piecewise quadratic defined on a triangular partition. In this case a contour line at height H passing through a triangle must be described by a conic section. Such a section can

be represented in parametric form as

$$x(t) = (b_0 + b_1 t + b_2 t^2)/(b_3 + b_4 t + b_5 t^2)$$

$$y(t) = (b_6 + b_7 t + b_8 t^2)/(b_3 + b_4 t + b_5 t^2),$$

see Powell [156]. Powell has promised an algorithm based on this observation.

We turn now to some methods for handling general functions f on arbitrary domains D.

8.4. A simple line-printer method. The following simple-minded method can produce reasonable-looking contours without excessive computation, and without recourse to a plotter. Suppose H is a rectangle enclosing the domain D, and that we partition H as $H = \cup H_{ij}$ with a rectangular grid as in (6.2). Let $HL < HU$ be given real numbers. Finally, suppose that t_{ij} is some point in H_{ij} where f can be evaluated (perhaps one of the corners or the center). Define

$$(8.3)\quad C_{ij} = \begin{cases} 0 & , \text{ if } f(t_{ij}) < HL \\ 9 & , \text{ if } f(t_{ij}) > HU \\ v & , \text{ if } HL + (v-1)h < f(t_{ij}) < HL + vh,\ 1 \le v \le 8, \end{cases}$$

for all $i = 0,1,\ldots,k$ and $j = 0,1,\ldots,l$ (where $h = (HU-HL)/8$). The $(k+2)$ by $(l+2)$ matrix C contains only integers, and if it is printed out without either horizontal or vertical spacing, we obtain a reasonable-looking contour map of the function. A typical example is included in Figure 7. The method can be refined by using an alpha-numeric array C and more than 10 symbols. It can also be refined by using a printer with appropriate horizontal spacing so that each symbol occupies a square rather than a rectangle (e.g., cf. Buneman [40]).

8.5. Threading on a rectangular grid. As in section 8.4.

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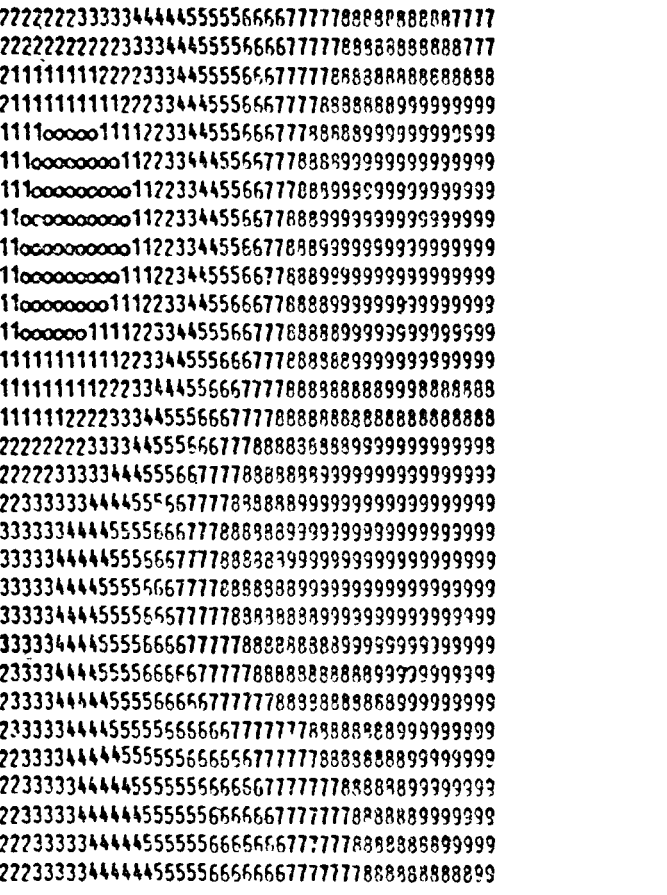

Figure 7. A Simple Contour Map (Heart Potential)

suppose that D is imbedded in a rectangle H which has been partitioned by a rectangular grid as in (6.2). Assuming that f is continuous, it is still possible to decide which of the grid lines a particular contour of height H crosses by examining the end-points of each such line. Since f is not generally linear along such a line, we cannot determine exactly where the crossing point is by linear inverse interpolation. However, if we are willing to evaluate f a few times along this line, we can estimate the crossing point quite accurately by bisection,

for example. Once a sequence of points on a contour has been determined, we may thread a curve through the points just as in section 8.2.

This method does have one serious drawback, however,--just as with the method discussed in section 8.2--, if we are tracing a contour it may happen that after entering a triangle there is an ambiguity as to which of two points to use to exit the rectangle. One could opt for an ad hoc rule or try the second-stage approximation described in section 8.2. For an example of how this method works, see Falconer [76] (based on Lodwick and Whittle [130]), where it is applied to a surface constructed by local weighted quadratic polynomial least-squares approximation. Since bisection is involved, one should realize that in drawing contours with this routine the surface f is going to be evaluated a great many times.

8.6. Threading on a triangular grid. An obvious cure for the ambiguity discussed in section 8.5 for threading on a rectangular grid is to use a triangular partition in the first place. Then the bisection method coupled with a threading routine leads immediately to a contouring routine for general surfaces f. Strangely enough, I have not been able to find anywhere where this method has been suggested.

I have made no effort to track down all available papers on contouring. A few which I did find and have not yet mentioned are Cottafawa and le Moli [60], Dayhoff [64], and Pelto et al [152]. There are many others.

In some cases it may be desirable to have a more graphic picture of a surface than a contour map can provide. Recently there has been considerable effort devoted to computer methods for displaying surfaces on a scope or with a plotter. For some examples of output and a discussion of methods, see e.g. the book by Barnhill and Riesenfeld [20] on computer-aided design.

If an actual 3-D picture is desired instead of just a perspective, it is even possible to produce holographs.

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C^1 Surface Interpolation For Scattered Data on a Sphere

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C^1 Surface Interpolation for Scattered Data on a Sphere

Abstract

This paper describes an algorithm for constructing a smooth computable function, f, defined over the surface of a sphere and interpolating a set of n data values, u_i, associated with n locations, p_i, on the surface of the sphere. The interpolation function, f, will be continuous and have continuous first partial derivatives. The locations, p_i, are not required to lie on any type of regular grid.

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C^1 Surface Interpolation for Scattered Data on a Sphere

1. Introduction

The problem of constructively defining a smooth surface that interpolates data defined at scattered points in the plane has been treated in different ways by a number of authors. For surveys of this work up to 1977 see Refs. (2) and (7).

We consider here the analagous problem for data defined at scattered points over the surface of a sphere. When data is defined over only a portion of the surface of a sphere it may be most reasonable to map that portion of the spherical surface to a planar region, using a C^1 mapping function, and treat the problem by an algorithm designed for the planar domain problem. However when the data is scattered over the whole surface, and it is desired to produce a C^1 interpolation function defined over the entire surface, it seems necessary, or at least very desirable, to deal with the problem directly in the spherical setting. In particular, there is no C^1 function that will map the entire surface of a sphere to a bounded planar region.

2. The problem

Let S denote the surface of the unit sphere in 3-space. Given points p_i, i=1, ..., n, the problem is to construct a computable function f, defined and having C^1 continuity over S, and satisfying the interpolation conditions

$$f(p_i) = u_i \quad \text{for } i=1, \ldots, n$$

2.1 Relevant properties of C^1 functions on S

A function of f defined on S is differentiable at a point p_0 in S if and only if there exists a 3-vector g_0 satisfying

$$(1) \qquad \lim_{\substack{\|dp\| \to 0 \\ p_0 + dp \in S}} \frac{f(p_0+dp) - (f(p_0) + g_0^T dp)}{\|dp\|} = 0$$

Let T_0 denote the tangent plane to the sphere at the point p_0. Since the perturbed points p_0+dp in Eq. (1) are required to lie in S, the normalized perturbation vectors $dp/\|dp\|$ approach the plane T_0 as $\|dp\|$ approaches zero. It follows that if a vector g_0 satisfies Eq. (1) then so also does any vector of the form g_0+h where h is orthogonal to the tangent plane T_0, i.e. where h is a multiple of the vector from the origin to p_0.

To resolve this nonuniqueness of vectors g_0 satisfying Eq. (1) we will standardize on the shortest such vector. This vector is distinguished among vectors g_0 satisfying Eq. (1) by the property of being orthogonal to the position vector from the origin to p_0, or equivalantly by the property that the point p_0+g lies in the tangent plane T_0. We will call this vector g_0 the <u>gradient</u> vector of f at p_0.

Note that the fact that f has a restricted domain, namely S, is an essential part of this definition. For example if f is the restriction to S of some function f defined in an open neighborhood of 3-space containing p_0 it is entirely possible that f may be differentiable at p_0 and have a unique gradient vector g that is different from the (minimal length) gradient vector g_0 of f. In such a case however g_0 will be the orthogonal projection of g onto the 2-D subspace parallel to the tangent plane T_0.

Let U be a region of S containing p_0 and not extending more than $\pi/2$ radians away from p_0 in any direction. Let k be the one to one mapping of points of U to their orthogonal projections in T_0. Let U_0 be the region in T_0 to which U is mapped by k. Define the function f_0 on U_0 by

$$f_0(s) = f(k^{-1}(s))$$

Note that the point p_0 is in both the domains of f and f_0. If f is differentiable at p_0 with gradient vector g_0 then also f_0 is differentiable at p_0 with gradient vector g_0. We will make use of this local equivalence of f and f_0 later in deriving an algorithm for estimating the gradient of f from discrete data.

We will say a function defined on S is in the class C^1 if there is a continuous 3-D vector-valued function g, defined on S, such that for each point $p_0 \in S$ $g(p_0)$ is orthogonal to the vector from the origin to p_0 and satisfies the condition ascribed to g_0 in Eq. (1).

3. Major steps of the solution method

The approach to be described has the same major steps as the method for the analagous planar problem given in Ref. (6). These steps are

1. Build a triangular grid on S having the given points p_i as vertices.

2. Estimate the gradient vector g_i at each point p_i.

3. To evaluate the interpolation function f at an arbitrary point p in S:

   (a) Look up p in the grid to find the triangle containing p.

   (b) Compute f(p) by an interpolation method using the given function values u_i and the estimated gradient vectors g_i at the three vertices of the enclosing triangle.

3.1 Data structures

In the algorithms to be described the points p_i will be represented by their cartesian coordinates. It will be convenient in the following to let the same symbol denote either a point or the 3-D vector from the origin to the point. In particular, points in S are represented by vectors of unit euclidean length.

Each triangle will have an index number and will be represented by a set of six pointers identifying the three adjacent triangles and the three vertex points. This is exactly the same data structure as was used in Ref. (6).

If triangle t has vertices whose indices are A, B, and C in counterclockwise order, and whose adjacent triangle indices are a, b, and c with triangle a opposite vertex A, b opposite B, and c opposite C, the six pointers

representing triangle t would be stored in one of the following three permutations:

a, b, c, B, C, A
b, c, a, C, A, B
c, a, b, A, B, C

All access to these pointers is done via three very short subroutines. Thus the actual storage mode for these pointers is "hidden" from the rest of the program. By appropriate programming of these three subroutines the pointers can be packed to save storage.

The array storage requirements of this algorithm are thus

- 3n locations for the vectors p_i, i=1, ..., n.
- n locations for the data values u_i, i=1, ..., n.
- 12n locations for the triangle pointers. This is based on 6 pointers per triangle and at most 2n-4 triangles. This storage requirement can easily be reduced by packing.
- 3n locations for the gradient vectors g_i, i=1, ..., n.
- n locations for a permutation vector used only while building the grid. This storage could be overlaid by the gradient vector array or could be eliminated entirely by minor changes in the program design.

3.2 Determinantal tests and grid look-up

Let p_1, p_2, and p_3 be 3-vectors having unit euclidean length. Let $\mathrm{Det}(p_1, p_2, p_3)$ denote the determinant of the 3x3 matrix whose column vectors are p_1, p_2, p_3 in that order.

If $\Delta = \mathrm{Det}(p_1, p_2, p_3) \neq 0$ then no two of the vectors form an angle of zero or π, and the three vectors do not all lie in a single plane through the origin. In this case a proper spherical triangle can be formed by connecting each of the three pairs of points by the shorter arc of the great circle in S determined by that pair of points. Thus each arc will have length less than π.

This triangle divides S into two regions. The smaller region is to be regarded as the interior of the triangle. If $\Delta > 0$ an observer traversing the edges of the triangle with the interior of the triangle to the left will visit the vertices in the order p_1, p_2, p_3. If $\Delta < 0$ the ordering would be reversed. We will always order the vertices of triangles so that $\Delta > 0$.

Let p_1, p_2, p_3, be vertices of a proper triangle t in S with $\Delta > 0$.

Regarding q as a variable 3-vector in S, note that the quantity

$$s_1 = \text{Det } (q, p_2, p_3)$$

is proportional to the distance of q from the plane determined by the vectors p_2 and p_3 with the sign of s_1 being positive if q is on the same side of the p_2p_3 plane as p_1 and negative if q is on the opposite side. Thus a point $q \in S$ is inside the triangle t if and only if the three quantities

$$s_1 = \text{Det } (q, p_2, p_3)$$
$$s_2 = \text{Det } (p_1, q, p_3)$$
$$s_3 = \text{Det } (p_1, p_2, q)$$

are all nonnegative.

Our algorithm for finding a triangle containing a given point q consists in computing the quantities s_1, s_2, s_3 for some triangle t and then either accepting t as the containing triangle if all $s_i \geq 0$ or else moving to the neighboring triangle across the edge opposite vertex p_i if s_i is the first of the test quantities found to be negative.

If there is no neighboring triangle across this edge the search stops, returning this information. Otherwise the search continues by computing the test quantities in the neighboring triangle.

Rounding errors in computing a 3x3 determinant causing inconsistent sign determination could conceivably lead to cycling in the look-up process or to the construction of topologically impossible edges in the grid construction.

Consider for example four points $p_1, \ldots, p_4$ that lie in order along an arc of a great circle, the arc having length less than π. The true mathematical value of the determinant of the 3x3 matrix formed using any three of these vectors is zero.

Using finite precision coordinates and finite precision floating point arithmetic these determinants will generally not be computed as zero. A nonzero result does not in itself cause a serious problem but the possibility of inconsistency in the evaluation of related determinants can.

To illustrate the hazard suppose that with $p_1, \ldots, p_4$ as above the computed value of $\mathrm{Det}(p_1, p_2, p_3)$ is positive and (p_1, p_2, p_3) is accepted as a triangle in the grid. Then suppose p_4 is tested for inclusion in this triangle. It is possible that all of the determinants $\mathrm{Det}(p_4, p_2, p_3)$, $\mathrm{Det}(p_1, p_4, p_3)$, and $\mathrm{Det}(p_1, p_2, p_4)$ might evaluate nonnegative. This would lead to the erroneous conclusion that p_4 is contained in the triangle (p_1, p_2, p_3) and various topologically incorrect edges would be constructed to incorporate p_4 into the grid.

Using a tolerance ϵ such that all results between $-\epsilon$ and ϵ are treated as zero does not solve the problem. We have had good luck using double precision evaluation of the determinants and strict zero tests. We have also had success with single precision determinant evaluation if we randomized the order in which the points p_i were considered for inclusion in the grid.

One way to assure consistency while sacrificing some accuracy would be to truncate all coordinate values to a small enough number of bits to permit the determinant evaluation to done exactly. For example, on a machine carrying fourteen hexadecimal digits of significance in a double precision number, one might round all coordinates to the 2^{-17} bit. The smallest nonzero bit that could occur in the product of three such numbers would be the 2^{-51} bit. The coordinates do not exceed one in magnitude so the same is true of their products. These products and the sum of up to six such products can be held exactly in a normalized floating point number carring fourteen hexadecimal digits. Thus determinants of 3x3 matrices could be computed exactly.

3.3 Constructing the triangular grid

The convex hull of a finite set of points in the plane is the smallest convex polygon containing the entire point set. We need an analagous notion, which we will call the spherical convex hull, for points on the surface S of the unit sphere.

Let P be a finite set of points in S. If there is no plane that strictly separates the origin from P, we will say the whole surface S is the spherical convex hull of P.

Alternatively if there is a plane strictly separating the origin from P let C be the smallest convex cone with its vertex at the origin and containing the set P. The intersection of C with S will be called the spherical convex hull of P. This region will lie strictly within some hemisphere of S.

A triangular grid with n vertices and covering all of S will have 2n-4 triangles. A grid that convers a spherically convex proper subset of S and has n vertices and b boundary edges will have 2n-b-2 triangles. Note that 2n can always be used as an upper bound on the number of triangles.

Our method of constructing a triangular grid using a given finite point set P in S as vertices will be a sequential process that alters a grid covering the spherical convex hull of some set of k points of P to obtain a grid covering the spherical convex hull of these k points plus one more.

Algorithms of this type can be divided into (at least) three subtypes

(a) First find the boundary points of the (spherical) convex hull of P and construct a triangular grid for these points. Then in the remaining sequential part of the algorithm each new point is known to lie in some triangle of the current grid.

(b) Preprocess the points of P into an ordering that assures that each new point will be strictly outside the (spherical) convex hull of the preceeding points.

(c) Do no prepreprocessing and be prepared for each new point to be either inside or outside the (spherical) convex hull of the preceeding points.

With subtypes (a) and (b) one is adding extra code and execution time for a preprocessing stage in the hope of permitting the subsequent sequential phase to be simpler and execute faster. We have at different times developed algorithms for the planar problem representing each of these subtypes. The algorithm of Ref.(6) is of subtype (b). My present inclination is to prefer subtype (c) as I think it permits the total program to be simpler and probably is not significantly slower if in fact it is any slower. More specifically it does not require storage for a separate data structure to keep track of boundary points as was the case in Ref. (6).

Our approach then is to form one initial triangle and then loop through the remaining n-3 points adding one at a time and modifying the triangular grid at each stage to cover the spherical convex hull of all the points so far considered. Each new point may be either inside or outside the grid so far constructed.

In the class of problems for which this method is primarily intended, i.e. problems in which the data is scattered quite generally over all of S, a stage will be reached at which the spherical convex hull is all of S. Thereafter all additional points will necessarily lie inside the grid so far constructed since the grid will cover all of S. The user can cause this full coverage of S to happen early by arranging that the first four points to be processed are located such that the tetrahedron with these four points as vertices contains the origin as a strictly interior point. The triangular grid based on these four points will cover all of S.

Initially the algorithm seeks three points with which to construct the first triangle. The first vector p_1 is accepted unconditionally. The remaining vectors are scanned for the first one whose inner product with p_1 lies between cos 179^o and cos 1^o, i.e. between -0.99985 and 0.99985. Pointers are swapped to relabel this vector as p_2.

The remaining vectors are scanned to find one whose determinant along with p_1 and p_2 exceeds 0.001 in magnitude. Such a vector is relabeled as p_3. The vectors p_2 and p_3 are then swapped if necessary to assure that $\mathrm{Det}(p_1, p_2, p_3)$ is positive. This completes the construction of the first triangle.

We may now assume a grid based on k-1 points has been constructed and the next point, p_k, is to be introduced. A look-up is done using the method described in Sec. 3.2. This look-up either finds a triangle t containing p_k, or else finds a triangle t such that p_k is outside this triangle relative to a side of the triangle beyond which there is no adjacent triangle.

In the first case, the single triangle t having vertex points p_A, p_B, p_C will be replaced by three triangles having vertex points (p_k, p_B, p_C), (p_A, p_k, p_C), and (p_A, p_B, p_k) respectively. The algorithm then does a grid improvement phase to be described subsequently.

In the second possible outcome of the look-up process, the point p_k is strictly outside the spherical convex hull of the preceeding k-1 points, and in particular it is outside an edge of triangle t that constitutes a portion of the boundary of the spherical convex hull. In this case one new triangle will be formed by connecting p_k to the two ends of the edge of t that gave a negative s_i value in the look-up testing (See Sec. 3.2).

The algorithm next scans the current grid boundary points in both directions from the new triangle and connects p_k to all other boundary points that result in the creation of proper spherical triangles (See Sec. 3.2). The algorithm then does grid improvement.

3.3.1. Grid improvement

When two adjacent spherical triangles form a strictly convex spherical quadrilateral there arises the possibility of replacing these two triangles by the two that occur when the quadrilateral is partitioned by its other diagonal. One must establish a criterion for choosing between the two possible disections of a quadrilateral.

This issue was discussed for the planar case in Ref. (6) where it was shown that three differently stated criteria were mathematically equivalent. In the spherical setting a fourth criterion with considerable intuitive appeal can be formulated and it is easily seen to be equivalent to the "circle test" of Ref. (5).

Let p_1, p_2, p_3, and p_4 be the vertices, in counterclockwise order, of a spherical quadrilateral in S. Assume all four of the potential triangles $(p_1\ p_2\ p_3)$, $(p_2\ p_3\ p_4)$, $(p_3\ p_4\ p_1)$, and $(p_4\ p_1\ p_2)$ would be proper spherical triangles. One choice would be to connect points p_1 and p_3 forming triangles $(p_1\ p_2\ p_3)$ and $(p_3\ p_4\ p_1)$ while the other choice would be to connect points p_2 and p_4 forming triangles $(p_2\ p_3\ p_4)$ and $(p_4\ p_1\ p_2)$.

Consider the 3-D polyhedron underlying the spherical triangular grid. If the four points under consideraton are not coplanar then one choice will give underlying planar triangular faces that could be faces of a convex polyhedron and the other choice will not. This therefore is our new criterion: a preference to make the underlying 3-D polyhedron convex.

Another way to describe this criterion is to consider the unique line L from the origin that intersects both of the lines p_1p_3 and p_2p_4. If p_1, p_2, p_3, and p_4 are not coplanar the two lines will intersect L at two distinct points. We construct the one of these two lines that intersects L furtherest from the origin.

We implement this test by computing $d = \text{Det}\ (p_2-p_1,\ p_3-p_1,\ p_4-p_1)$ and constructing the line p_2p_4 if $d > 0$ and constructing p_1p_3 if $d < 0$. Either line can be used if $d = 0$.

After a new point, say p_k, is connected into the grid, each edge that is opposite p_k in some triangle is a candidate for swapping. Thus if there is a triangle $p_kp_2p_4$ and an adjacent triangle $p_2p_3p_4$ the edge p_2p_4 will be replaced by the edge p_kp_3 if $\text{Det}\ (p_2-p_k,\ p_3-p_k,\ p_4-p_k)$ is negative. When an edge is swapped the edges opposite p_k in the two newly formed triangles become candidates for swapping.

3.4. Estimation of gradient vectors

We assume a triangular grid has been constructed in S covering the spherical convex hull of the points $p_1, \ldots, p_n$ and having the points $p_1, \ldots, p_n$ as vertices. We also assume the data values $u_1, \ldots, u_n$ (See Sec. 2) are available. It is required to estimate a 3-D gradient vector g_i at each point p_i. See Sec. 2.1 for the characterization of gradient vectors for this problem.

Let p_i be a point at which a gradient vector g_i is to be estimated. Our general idea is to do a least squares quadratic fit to data near the point p_i and then use the gradient vector of this fitted quadratic polynomial as the gradient vector at p_i. We use a six term quadratic polynomial in two variables forcing interpolation to the value u_i at p_i. Thus we need at least five neighboring points, and prefer more than five to obtain a local smoothing effect on the gradient vector.

Let Q denote the set of points to be used for the fit. We first place all the immediate neighbors of p_i into Q. If the number of immediate neighbors is

from 6 through 16 and if the maxtrix for the least squares problem passes a conditioning test then this set Q is used for the fit. If the number of points exceeds 16, excess points are discarded. If the number is less than 6, more nearby points beyond the immediate neighbors of p_i are introduced. If the matrix condition test is not passed, more points, up to 16, are added. If the condition test still fails with 16 points, the least squares system is damped to bias the solution toward small values of the coefficients of the three second order polynomial terms.

The fitting is set up in a local coordinate system determined by p_i. A 3x3 rotation matrix R is determined that transforms the position vector of p_i to the vector (0, 0, 1). Thus the "north pole" of the rotated coordinate system is at p_i.

The same coordinate transformation is applied to all vectors in the fitting set Q. Generally these transformed vectors, having some proximity to p_i, will all lie in the "northern hemisphere" of the rotated coordinate system i.e. their z coordinates will be positive. If any transformed vector (x,y,z) has $z < 0$ we arbitrarily replace it by (x/s, y/s, 0) where $s = \text{Sqrt}(x^2 + y^2)$. This last step is just an expedient to do something definite in a poor situation. Data must be very sparse or poorly distributed to result in any points of Q being in the "southern hemisphere" of the rotated coordinate system.

We ignore the z coordinates of these transformed vectors, using only their x and y coordinates in the fitting. This can be interpreted as projecting the points p_j of Q orthogonally onto the plane T that is tangent to the sphere at the "north pole", i.e. at p_i. The polynomial model for the fit is

$$c_1x + c_2y + c_3x^2 + c_4xy + c_5y^2 = u-u_i$$

The coefficients $c_1, \ldots, c_5$ of this polynomial are determined by a least squares computation. The 2-vector (c_1, c_2) is the gradient vector at p_1 of the fitted polynomial relative to the xy coordinate system in the tangent plane T. Using the observations at the end of Sec. 2.1 we take the 3-vector $(c_1, c_2, 0)$ to be the gradient vector at p_1 of the (as yet unknown) interpolating function defined over the surface of the sphere. The inverse of the rotation matrix R is then applied to $(c_1, c_2, 0)$ to obtain the representation of the gradient vector g_1 in the original coordinate system.

3.5. Interpolation in a single triangle

In the planar case described in Ref. (6) we preferred the 9-parameter Clough-Tocher cubic macroelement (Ref. 3) as our interpolation method primarily for the following two reasons:

(a) It is more economical to evaluate than any other C^1 interpolation method of which we are aware. Beginning with the rectangular coordinates of q and of the vertices, and the function values and 2-D gradient vectors at the vertices, our evaluation of this interpolant uses 55 multiplies, 65 adds, and 4 divides.

(b) The interpolant at any point is simply a cubic polynomial in the cartesian coordinates (or in the barycentric coordinates), and thus it is easy to derive and implement an evaluation of the gradient of the interpolated surface if this should be desired.

Unfortunately, the Clough-Tocher method depends strongly on properties of polynomials in cartesian coordinates over a planar region and does not seem to generalize for use over a spherical triangle.

We will describe two methods for C^1 interpolation over planar triangles that do generalize to spherical triangles. These both represent the interpolant in the form

$$f(q) = w_1 f_1 + w_2 f_2 + w_3 f_3, \qquad w_1 + w_2 + w_3 = 1 \tag{2}$$

where the w_i's are nonnegative weight functions depending only on q and the locations of the vertices, and the f's are interpolants depending in general on q and all of the data associated with the triangle t, and satisfying some, but generally not all, of the conditions for C^1 continuity across triangle edges. A very helpful analysis of convex combination formulas of this type is given in Ref. (4).

As with the Clough-Tocher interpolant the requirement for C^1 continuity across edges is approached by establishing values of the function and its gradient along an edge that depend only on data at the two ends of the edge.

Values along an edge are computed by Hermite cubic interpolation and the tangential derivative at any point on an edge is computed as the derivative of this Hermite cubic interpolation polynomial. The normal derivative at any point on an edge is computed by linear interpolation using the derivatives normal to the same edge at the two ends of the edge. For q on an edge of a triangle to let F(q) denote the value and G(q) denote the gradient vector defined by these interpolation methods along the edge.

3.5.1. Planar Method 1

For any point q in the triangle t let f_1 in Eq. (2) be defined by Hermite cubic interpolation along the line through q parallel to the edge opposite vertex p_i. This function f_1 has been called the BBG interpolant or BBG projector due to its use in Ref. (1). See also Ref. (2), pp. 92-101.

Function and derivative values for this interpolation are derived from the edge functions F and G defined above. The function $f_i(q)$ defined in this way is C^1 over triangle t, and f_1 and its gradient match F and G respectively on all edges except that the normal derivative of f_i on the relative interior of the edge opposite p_1 will generally not be consistent with G.

Corollary 2.5 of Ref. (4), adapted to our present notation, states that if all f_i's in Eq. (2) match F on the entire boundary of t, and $w_1(q) = 0$ for any 1 and edge point q for which the gradient of f_1 evaluated at q does not match G(q), then f of Eq. (2) matches F and the gradient of f matches G on the entire boundary of t.

Thus letting f_1 be the BBG interpolant, it will suffice to require that w_1 have the value zero on the edge opposite p_1 and be nonzero elsewhere on the boundary of t. This is conveniently assured by letting w_1 be the barycentric coordinate of q that has the value zero on the edge opposite p_1 and one at p_1. Thus Eq. (2) specializes to

$$f(q) = b_1 f_1(q) + b_2 f_2(q) + b_3 f_3(q) \tag{3}$$

where the b_1 are the barycentric coordinates of q relative to the triangle t and the f_1's are BBG interpolants, each requiring two linear interpolations and three Hermite cubic interpolations for its evaluation.

3.5.2. Planar Method 2

For any point q in the triangle t let f_1 in Eq. (2) be defined by Hermite cubic interpolation along a line from vertex p_1 through q to the opposite edge. This interpolant has been called a side-vertex or radial interpolant. (See Ref. 2, p. 101).

The function f_i matches F on the entire boundary of t and its gradient matches G on the edge opposite p_i but its normal derivative is not consistent with G_i on the relative interior of the two edges adjacent to p_i. Again using Corollary 2.5 of Ref. (4), it suffices to define w_i of Eq. (2) to be zero on the relative interior of the two edges adjacent to p_i and positive on the relative interior of the opposite edge. This is accomplished by setting

$$w_i = b_{i+1}\, b_{i+2}/(b_{i+1}\, b_{i+2} + b_{i+2}\, b_i + b_i\, b_{i+1})$$

where the b_i's are barycentric coordinates of q and the subscripts are to be evaluated modulo 3 to one of the values 1, 2, or 3.

The function w_1 defined in this way has non-removable singularities at vertices p_{i+1} and p_{i+2} since it is one on the relative interior of edge $p_{i+1}p_{+2}$ and zero on the relative interior of the other two edges (and at vertex p_1). For mathematical definiteness we may define w_1 to have the value zero at p_{i+1} and one at p_{i+2}. The sum $w_1 + w_2 + w_3$ is then one throughout triangle t, as is required for Corollary 2.5. In a computer implementation one would treat interpolation at a vertex as a special (trivial) case anyway, so the particular choice of definition of w_i at the p_{i+1} and p_{i+2} has no bearing on implementations.

Thus Eq. (2) specializes to

(4)

$$f(q) = \begin{cases} (b_3b_2f_1 + b_1b_3f_2 + b_2b_1f_3)/(b_3b_2 + b_1b_3 + b_2b_1), & \text{for } q \neq p_1,\ p_2,\ \text{or } p_3 \\ u_i, & \text{for } q = p_i \end{cases}$$

where the b_i's are the barycentric coordinates of q and the f_i's are side-vertex interpolators. Each f_i requires one linear interpolation and two Hermite cubic interpolations for its evaluation.

3.5.3. Generalization of Planar Methods 1 and 2 for spherical triangles

The key in generalizing these two planar methods for use with a grid of spherical triangles on the surface S of the unit sphere is to replace all of the linear and Hermite cubic interpolations along line segments by the same type of interpolations along arcs of great circles in S.

Let t denote a proper spherical triangle with vertex position vectors p_1, p_2, and p_3, and let q be a point of S contained in t. Let t' denote the underlying planar triangle having the same vertices as t, and let q' be the central projection of q into the plane of triangle t', i.e. q' is the point in the plane of t' intersected by the line from the center of the sphere to q.

When the look-up procedure of Sec. 3.2 finds that a given point q in S is in triangle t, it also returns the three nonnegative numbers s_1, s_2, and s_3. We call these numbers unnormalized barycentric coordinates since the (normalized) barycentric coordinates of q' relative to the planar triangle t' can be computed as

$$b_i = s_i/(s_1 + s_2 + s_3), \quad i = 1, 2, 3.$$

The intersection points between certain lines through q' and edges of t' needed for either of the two planar interpolation methods are easily represented in terms of the b_i's and p_i's. Thus the intersection between edge p_ip_{i+1} with the line through q' parallel to edge $p_{i+1}p_{i+2}$ has position vector $b_ip_i + (1-b_i)p_{i+1}$ while the intersection between edge $p_{i+1}p_{i+2}$ with the line from vertex p_i through q has the position vector $(b_{i+1}\, p_{i+1} + b_{i+2}\, p_{i+2})/(b_{i+1} + b_{i+2})$.

These intersection points can then be centrally projected to S by normalizing their position vectors to have unit euclidean length. All of the linear and cubic interpolations called for in the planar methods are then done with respect to arc length along great circle arcs in S obtained by central projection of the corresponding line segments in the planar triangle t'.

Recall that gradient data at each vertex p_1, p_2, and p_3 is represented as a 3-vector that is orthogonal to the position vector of the vertex. Gradient information generated at auxiliary points in either interpolation method is also represented a 3-vector orthogonal to the associated position vector.

The verification that each of these two spherical triangle interpolation methods defines a C^1 function over S can be carried out in the same way the C^1 property of the planar methods is proved, for example in Ref. (4). Thus one observes that the function value and gradient vector at any edge point of a spherical triangle is determined only by data at the ends of the edge and thus will be consistent in neighboring triangles. The partial interpolation functions f_i have the correct values at all edge points and gradient values that are correct on certain edges and wrong on others. The convex combination formula (3) or (4) properly zeros out the functions where their gradient values are wrong and thus gives a function having the required boundary values and boundary gradients.

4. Software implementing these algorithms

Subroutines were written for these algorithms in 1979 using the JPL SFTRAN3 structured Fortran language which is preprocessed Federal (ANSI) Standard Fortran 77.

The time for grid construction for n points was proportional to $n^{1.25}$ for test cases in the range from 25 to 500 points. The RMS error in test cases using simple mathematical functions to generate data over relatively uniform triangular grids of various densities was proportional to $h^{3.4}$ in test cases having maximum edge length in the grid ranging from 63^0 down to 9^0.

A count of the number of arithmetic operations required to do a single interpolation in a triangle gives the figures listed in Table 1. The planar Clough-Tocher method is included for comparison. For all methods the computation starts with cartesian coordinates for q, p_1, p_2, and p_3 and function values and gradient vectors at p_1 p_2, and p_3. The weights used to combine the counts are arbitrary but plausible. They are normalized to cause an add plus a multiply to sum to one for consistency with operation counts measured in "Flops".

For Method 1, tests of the continuity of the interpolated function and its first partial derivatives across edges of the grid were made in two ways. Interpolated values and their first and second differences were computed at a sequence of equispaced points along a smooth arc. Paths were chosen crossing edges at various angles and crossing a vertex. These tests indicated continuity of the values and first differences with discontinuity of the second difference at edges.

The other test of C^1 continuity involved reprogramming all of the code for Method 1 using a "U-arithmetic" package developed at JPL in 1971 based on the ideas of Ref. (8). (This is like the method of Ref. (5) without the benefit of a preprocessor.) In this approach the program computes a 3-D gradient vector and a 3x3 Hessian matrix for every intermediate quantity and thus also for the final interpolated value. All derivative computations use mathematically correct formulas, i.e. not differencing.

We found it necessary to reorder some computations to avoid severe artificial numerical instabilities in the derivative computations. After this reordering the results were consistent with C^1 continuity.

We did not try a U-arithmetic version of Method 2. I would expect severe difficulties with this since the singularities of the w_i's at certain vertices (See Sec. 3.5.2) imply that some first partial derivations of the w_i's can be arbitrarily large in a small neighborhood of a vertex. Mathematically these cancel out but numerically there would be large rounding errors.

5. An application

In February, 1982, this software was used at JPL in the study of gravity variation over the surface of the planet Venus. Data was available at many, but not all points, of a rectangular longitude-latitude grid. The missing data occurred in irregularly shaped regions determined by geometrical constraints of the observation and communication instruments.

Table 1. Operation counts for a single interpolation in a triangle

	Clough-Tocher Planar Method	Spherical Method 1	Spherical Method 2	Factors for weighted total
Add/Subtract	65	371	352	0.4
Multiply	55	699	450	0.6
Divide	4	81	57	1.2
Sqrt		24	15	3.0
Atan		18	12	5.0
Weighted Total (Flops)	63.8	827.0	584.2	

Using 2450 points at which data was present our program built a spherical triangular grid consisting of 4896 triangles. Missing data in the rectangular grid was then filled in by interpolation in the triangular grid.

In the course of this work the scientists gained new insights regarding their data and we found and repaired a weak spot in our program. See the discussion of determinant evaluation in Sec. 3.2.

6. Conclusions and remarks

The efficiency of the grid building procedure, execution time in test cases being observed to be proportional to $n^{1.25}$, is quite satisfactory.

C^1 interpolation in a spherical triangle requires 9 to 13 more Flops than C^1 interpolation in a planar triangle. Modifications giving small reductions in the operation counts are known but it would be interesting if an entirely different approach could be found that might be more intrinsically related to the topology of the spherical surface and require significantly fewer Flops.

Method 1 is more time-consuming than Method 2 by a factor of about 3 to 2 since Method 1 uses nine cubic interpolations along arcs compared with six for Method 2. Analytic computation of gradients for interpolated values would probably be more stable using Method 1 than Method 2 because of the singularities in the w_i's of Method 2. It would be interesting to make visual comparisons of surfaces generated by these two methods but we have not had the resources to make such comparisons.

The programs appear to be robust and reliable. The use of the SFTRAN3 structured Fortran language has been extremely helpful in keeping the code understandable.

It should be noted that the use of the surface of a sphere as the domain is just a mathematical construct for dealing with the set of all directions in 3-space from an origin point. Thus the methods of this paper are applicable to the representation of any bounded two-dimensional C^1 surface in 3-space that is "starlike" in the sense that there is some origin point from which a ray in any direction intersects the surface in at most one point and the ray is not tangent to the surface at that point.

Other two dimensional manifolds besides the plane and the spherical surface that may deserve investigation for scattered data interpolation include the surface of a cylinder or a torus. On a cylinder one may wish to admit triangles having two vertices at the same data point while on the torus one may admit triangles having all three vertices at the same data point!

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D4

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SURFACES: Representation and Approximation

The general: Surface Application

Free-form Sculptured

Design of Surfaces

Representation of Surfaces

Examples:

Lockheed
Energy

Criteria/characteristics:

Fits given information/application

Smoothness

Shape fidelity

Parametric representation

Local vs. global schemes

Interactive design

Interactive viewing

NSF MCS-8101854

Outline of 3D Surfaces

Surfaces:

Interpolation v. Approximation

↓ ↓

Patches v. Points → Least Squares (J. G. Hayes, NPL)

↓ → Shepard's Formula

Coons v. Bezier → (2) Δ patches

↓

(1) □ patches → Preprocessors:

↓

Transfinite

- Boolean sums/correction surfaces
- Lofting interpolants
- Compatibility conditions

Discretization → Point methods

1. Triangulation
   - 1st pass
   - Optimization
2. Gradient specification

Triangular Interpolants

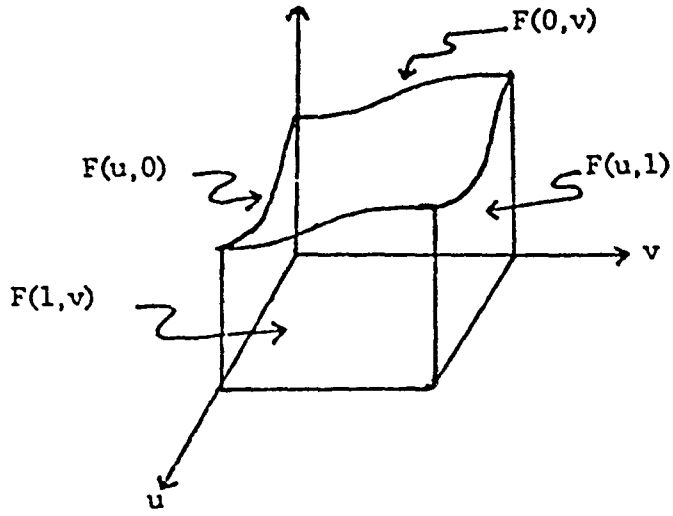
- Barycentric coordinates
- BBG
- Radial Nielson
- Symmetric Gregory
- Convex combinations

(1) □ Coons' Patches

S. A. Coons 1964

First Problem: Interpolate

to the 4 curves.



Conventions:

F "primitive"

F general coordinate

$\begin{bmatrix} x(u,v) \\ y(u,v) \\ z(u,v) \end{bmatrix}$ ← parametric surface

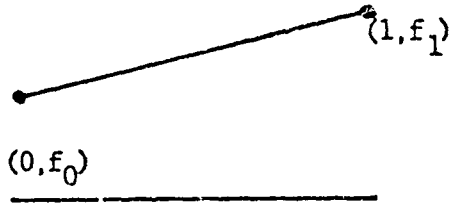
Solution to the 1st problem: Lofting interpolant

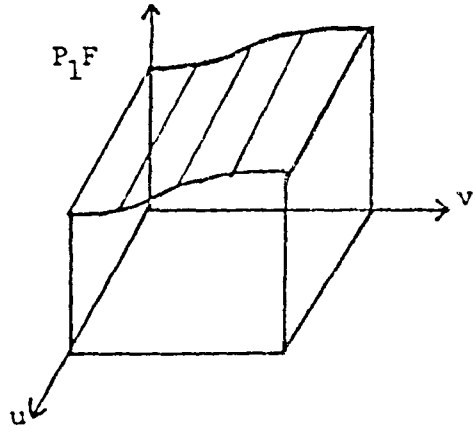
$P_1F \equiv (1-u)F(0,v) + uF(1,v)$

Univariate linear interpolant:

$f = f(u) \rightarrow P_1f = (1-u)f_0 + uf_1$.

Bivariate $F = F(u,v) \rightarrow P_1F$ = the above.





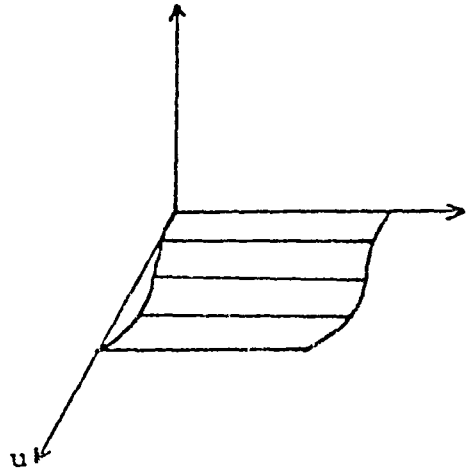
Error $F - P_1F$

Idea: Match. $F - P_1F$

and add this to P_1F .

Solution: $P_2[F - P_1F]$

does the job.



Geometry vs. Algebra

$g = g(v) \Rightarrow P_2 g = (1-v)g_0 + vg_1$

$\therefore P_2(F - P_1F) = (1-v)(F - P_1F)(u,0) + v(F - P_1F)(u,1)$

$= (1-v)F(u,0) - (1-v)[(1-u)F(0,0) + uF(1,0)]$

$+ vF(u,1) - v[(1-u)F(0,1) + uF(1,1)]$.

Overall approximation $PF = P_1F + P_2F - P_1P_2F$

$= (1-u)F(0,v) + uF(1,v) + (1-v)F(u,0) + vF(u,1)$

$- [(1-u)(1-v)F(0,0) + u(1-v)F(1,0) + (1-u)vF(0,1) + uvF(1,1)]$.

Check interpolation: $(PF)(u,0) = F(u,0)$ etc.

$PF = (P_1 \oplus P_2)F$ Boolean sum , transfinite interpolant, blending functions
W. J. Gordon 1969

P_1P_2F tensor product

Bilinearly blended Coons' patch

Piecewise method - C^0

Practical applications: C^1 or C^2 .

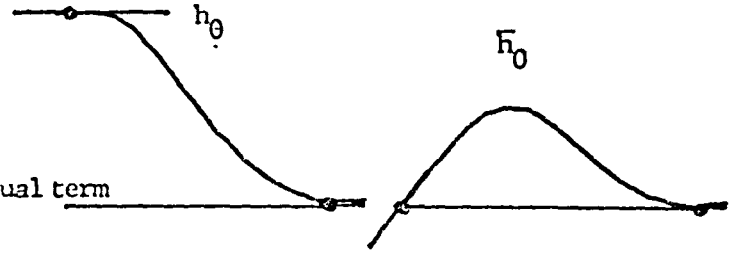
↳ ... bicubically blended Coons' patch.

$$f = f(u) \rightarrow P_1 f = h_0(u)f(0) + h_1(u)f(1) + \bar{h}_0(u)f'(0) + \bar{h}_1(u)f'(1)$$

$$F = F(u,v) \rightarrow$$

$$(P_1 \oplus P_2)F =$$

$$[h_0(u)h_1(u)\bar{h}_0(u)\bar{h}_1(u)]\begin{bmatrix} F(0,v) \\ F(1,v) \\ F_{1,0}(0,v) \\ F_{1,0}(1,v) \end{bmatrix} + \text{dual term}$$



$$- [h_0(u)h_1(u)\bar{h}_0(u)\bar{h}_1(u)]B\begin{bmatrix} h_0(v) \\ h_1(v) \\ \bar{h}_0(v) \\ \bar{h}_1(v) \end{bmatrix} \quad \text{where}$$

$$B = \begin{bmatrix} F(0,0) & F(0,1) & F_{0,1}(0,0) & F_{0,1}(0,1) \\ F(1,0) & F(1,1) & F_{0,1}(1,0) & F_{0,1}(1,1) \\ F_{1,0}(0,0) & F_{1,0}(0,1) & F_{1,1}(0,0) & F_{1,1}(0,1) \\ F_{1,0}(1,0) & F_{1,0}(1,1) & F_{1,1}(1,0) & F_{1,1}(1,1) \end{bmatrix} = \left[\begin{array}{c|c} F & F_{0,1} \\ \hline F_{1,0} & F_{1,1} \end{array}\right]$$

Twist trouble ("$F_{1,1}$" $\equiv \frac{\partial^2 F}{\partial u \partial v}$) $= \left[\begin{array}{c|c} \text{Positions} & \text{Tangents} \\ \hline \text{Tangents} & \text{Twists} \end{array}\right]$

Gregory's Square $\left[\begin{array}{c} \dfrac{u\frac{\partial^2 F}{\partial v \partial u}(0,0) + v\frac{\partial^2 F}{\partial u \partial v}(0,0)}{u+v} \\ \cdot \end{array} \quad \cdot\right]$

Discretization → Point Methods

$$F(u,0) \approx \tilde{F}(u,0) \equiv h_0(u)F(0,0) + h_1(u)F(1,0) + \bar{h}_0(u)F_{1,0}(0,0) + \bar{h}_1(u)F_{1,0}(1,0)$$

2. Triangular Patches

Rectangular domains vs. non-rectangular domains

Preprocessors: a. Triangulation

Algorithm: (1) Enforce given boundary

Default: convex hull.

(2) A triangulation ... fast.

(3) Optimize: $\min_{T} \max_{T \in T}$ angle

where T is the set of triangulations.

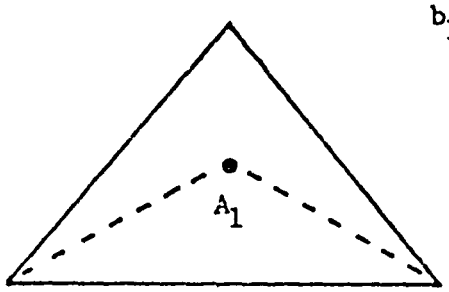
b. Gradient Specification

Surface Design: use tangent handles

Surface Representation: use triangular Shepard's Method (Little) or inverse-distance-weighted least squares (Franke).

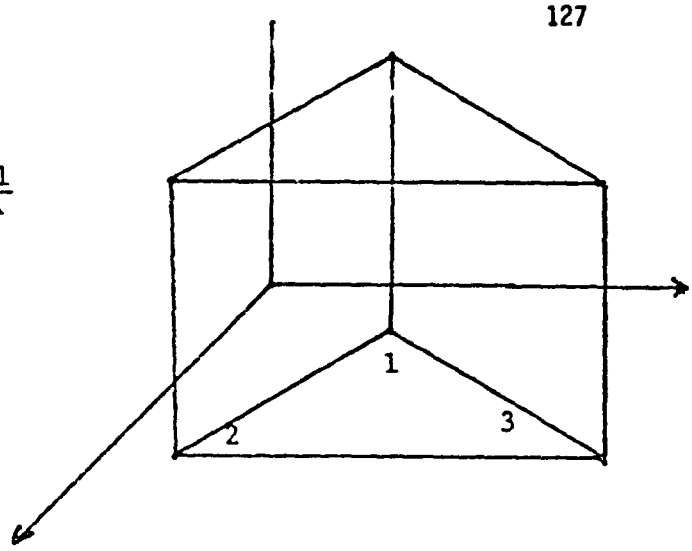
Triangular Interpolants

Barycentric coordinates



$$b_1 = \frac{A_1}{A}$$

etc.



Linear interpolant $LF = b_1F(V_1) + b_2F(V_2) + b_3F(V_3)$

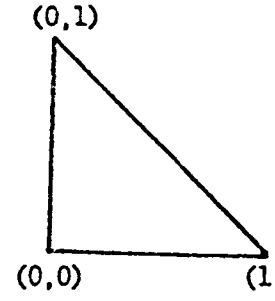
(Finite elements)

Problem: Find C^1 triangular interpolants

C^1 triangular Coons' patches

Barnhill, Birkhoff, Gordon, 1969-73

Standard triangle



The BBG idea: Loft & Boolean sum

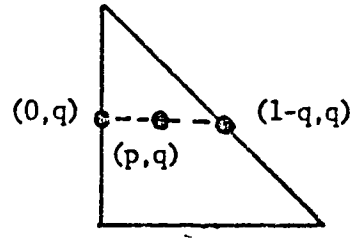
$$P_1F = h_0(\tfrac{p}{1-q})F(0,q) + h_1(\cdot)F(1-q,q)$$

$$+ \bar{h}_0(\cdot)(1-q)F_{1,0}(0,q) + \bar{h}_1(\cdot)(1-q)F_{1,0}(1-q,q)$$

Heuristic only: use modern version in practice.

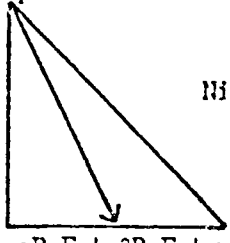
P_2F is analogous.

Form $(P_1 \oplus P_2)F$. Compatibility conditions



More triangular interpolants:

Radial



Nielson 1971

Symmetric Gregory scheme $\alpha P_1F + \beta P_2F + \gamma P_3F$

BBG projectors

α, β, γ polynomials from the Birkhoff Pit.

Convex Combination $\hat{\alpha}T_1F + \hat{\beta}T_2F + \hat{\gamma}T_3F$

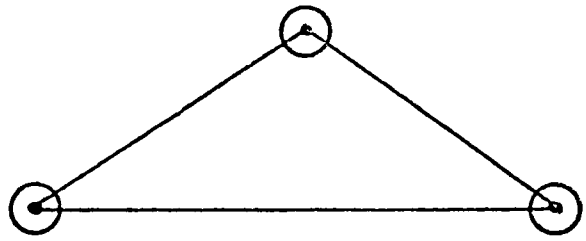
T_iF C^1 interpolant on edge i

Brown
Little

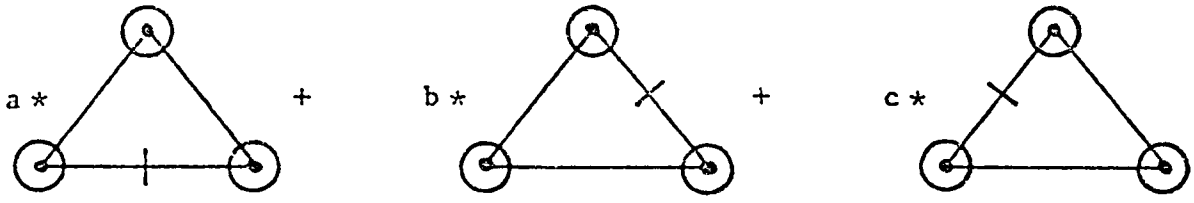
$\hat{\alpha}, \hat{\beta}, \hat{\gamma}$ rational functions from Shepard's Formula.

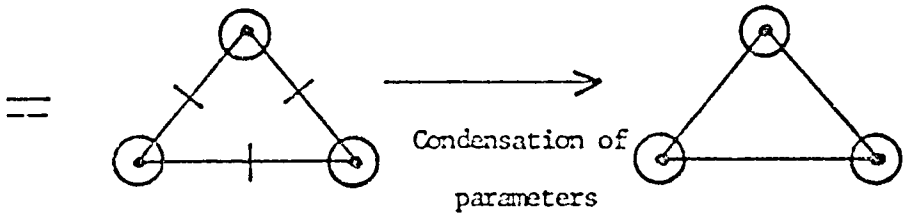
Finite dimensional triangular schemes:

C^1: User supplied data



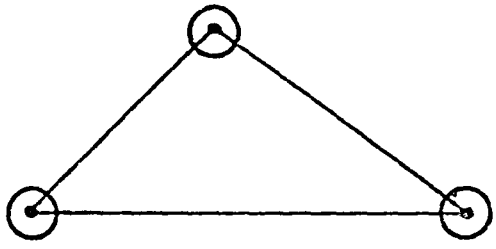
(1) Little Triangle (1976)



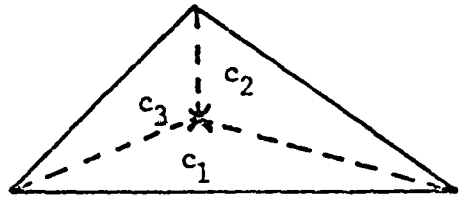


Rational, almost polynomial.

(2) C^1 Clough-Tocher piecewise cubic



User-supplied data



Clough-Tocher subdivision

Problem: Find C^2 Clough Tocher.

Tool: Farin's Bézier Triangle methods 1979.

Solution: Barnhill, Farin, and Little 1980.

Contouring: This is sometimes the problems, e.g., hidden surfaces, silhouette edges.

Adaptive subdivision schemes	Little Petersen

Point Methods: Arbitrarily Spaced Data

Shepard's Formula (1968) Solar maps

$$(SF)(x,y) = \begin{cases} \dfrac{\sum_i \dfrac{F_i}{d_i^2}}{\sum_i \dfrac{1}{d_i^2}} & (x,y) \neq (x_i,y_i) \ \forall_i \\ F_j & (x,y) = (x_j,y_j) \end{cases}$$

where $d_i = d_i(x,y)$ = distance from (x,y) to (x_i,y_i) .

Rewrite $$SF = \frac{\sum_i \left(\prod_{k \neq i} d_k^2 \right) F_i}{\sum \left(\prod_{k \neq i} d_k^2 \right)} \equiv \sum_i w_i F_i$$

where $$w_i(x_j,y_j) = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} ,$$ cardinal form.

$\therefore$ SF interpolates and is continuous.

Global method / flat spots

Improvements: Barnhill & Poeppelmeier 1975

Franke 1975

Vittitow 1978

Little 1978

Remarks: Patch methods are local methods.

Shape fidelity requires at least local quadratic precision.

Interactive design - real time computations.

Interactive viewing - use the hardware.

Reference: R. E. Barnhill, Representation and Approximation of Surfaces, Math. Software III, J. R. Rice, ed., Academic Press, 1977.

4D Surfaces — Example: Temperature as a function of 3 spatial variables.

Tessellation of 3D domains into tetrahedra. — Little

↓

4D Surface Interpolants — Gregory, Mansfield

↓

3D Contours — Jensen

D5

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SURFACE FITTING WITH BIHARMONIC AND HARMONIC MODELS

Rolland L. Hardy

May 1982

This paper was prepared for presentation to the
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Texas A&M University, College Station, Texas 77843
May 1982

SURFACE FITTING WITH BIHARMONIC AND HARMONIC MODELS

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BIOGRAPHICAL SKETCH

Rolland L. Hardy is Professor in Charge of a graduate degree program in Geodesy and Photogrammetry and of an undergraduate degree program in Surveying at Iowa State University. After leaving military service as a First Lieutenant, Field Artillery in 1946, he received a BS degree at the University of Illinois in 1947. The B.S.C.E. and C.E. degrees were obtained at the University of Missouri School of Mines at Rolla in 1950 and 1956 respectively. In 1963 he earned the degree of Dr.-Ing. (in Geodesy) at the Technical University, Karlsruhe, Germany. He is a registered professional engineer and surveyor in Iowa and Missouri. His career in surveying and mapping has included military and government service, both foreign and domestic, as well as private practice, teaching and research. He is in the retired reserve at the rank of Lieutenant Colonel, Corps of Engineers. Dr. Hardy is listed in American Men of Science and Who's Who in Engineering.

BACKGROUND

This paper is devoted mainly to a physical and geometric interpretation of the surface fitting technique discovered by the author in 1968, which was called multiquadric equations in 1971 (Hardy 1971). It was not until 1980, after a report by Franke (1979) that it was recognized that multiquadric equations or MQ may be interpreted very simply as a linear combination of three dimensional distance functions. The similarity of the MQ method to a simple summation associated with point mass models in geodesy was recognized very early (Hardy 1972). As it turns out now this was simply the other side of the biharmonic-harmonic "coin", and I have recently coined a multiquadric label for the point mass anomaly also, i.e. reciprocal multiquadric or MQ^{-1}. In this case we construct a set of point mass anomalies having positive and negative values as contrasted with always positive masses. By requiring or assuming the sum of mass anomalies to total zero we do not change the total mass and are therefore dealing with irregularities in a distribution of mass with respect to what we perceive to be some standard distribution of mass. For disturbing potential outside the anomalous masses we obtain a solution with a linear combination of three dimensional reciprocal distance functions, in which the originally unknown point mass anomalies are treated as undetermined coefficients. A reciprocal distance function is harmonic, satisfying Laplace's differential equation. Hence, a linear combination of such functions is also harmonic. An alternative way of looking at the problem and its solution is to consider the integral

$$T(r_p,\theta_p,\lambda_p) = G\iiint_{\text{Sphere}} \ell^{-1}(r_p,\theta_p,\lambda_p;r,\theta,\lambda)\, dm$$

in which p is a point on or outside the spherical body where disturbing potential T is measured. This integral cannot be formally integrated because the equality $dm = \delta(r,\theta,\lambda)\, dv$ contains an unknown density function $\delta(r,\theta,\lambda)$ under the integral sign. Therefore the integral, considered in this light, has the characteristics of an integral equation. Jaswon and Symm (1977) have studied problems of this type in both potential and elasticity. It is this form of a numerical approximation to a linear integral equation which provides a solution for the anomalous density function using MQ^{-1}. Measurements of disturbing potential at n points and the formation of a system of up to n linear equations provides the fundamental basis of this approach. However, the approximation of the density function is not the primary goal usually. After obtaining a good approximation of the density function it is used in the summation form to evaluate T at any point, usually where T has not been measured. The ultimate outcome then, is a procedure that one can classify as prediction, approximation, or surface fitting, if not some other form of numerical analysis.

A frequent problem with MQ^{-1}, or point mass models in general, is to find the best depth or radius for placing the anomalies. Hardy (1978, 1979) and Hardy and Gopfert (1975) have provided a very satisfactory solution for

this with respect to both spheres and planes. This is the "best-r formula", but it does not seem to be well known. The original MQ form (now known to be biharmonic) is relatively insensitive to this problem, and as noted by Franke (1979) it seems to give results equal to or better than MQ^{-1} for most surface fitting purposes. Hence MQ essentially as used in 1971, will probably become the favorite of the two surface fitting techniques.

The emphasis below will be on MQ rather than MQ^{-1} but contrasts and similarities of the two will be shown. As will be seen, it is the geometric and physical interpretation that has been applied to MQ^{-1} which has contributed to a better understanding of MQ. To summarize briefly in advance:

(1) MQ^{-1} is harmonic; MQ is biharmonic.
(2) MQ^{-1} deals basically with exterior disturbing potential and satisfies Laplace's equation; MQ deals basically with interior and surface displacements, elastically, and satisfies Poisson's equation.
(3) In both cases the solutions may be viewed as being numerical approximations of an integral equation in which an unknown density function is the physical source for disturbing potential (MQ^{-1}) or elastic displacement (MQ).

Most of what follows has been taken quite literally from my recent papers (Hardy 1980,1981). There has not been a rapid expansion of my knowledge on the subject since 1980; however, I am taking advantage of this opportunity to remedy a few misleading statements, to correct outright mistakes, and to change other matters, particularly Figure 2 which represents the elastic displacement of a sphere. Hence what is presented is considered to be a modest improvement over my previous papers.

BIHARMONIC-HARMONIC MODELS FOR SURFACE FITTING

Recognition that MQ is biharmonic in three dimensions, just as MQ^{-1} is harmonic in three dimensions, was expedited by Franke's (1979) description of Duchon's thin plate spline or TPS. Franke noted similarities of TPS and MQ in the fact that ordinates for a single kernel function get larger in both cases as the distance increases. TPS involves a biharmonic function in two dimensions of the form:

$$r^2 \log r \text{ with } r = (x^2+y^2)^{\frac{1}{2}}$$

whereas MQ involves a biharmonic function in three dimensions of the form:

$$r^2 \cdot r^{-1} \text{ or simply } r \text{ with } r = (x^2+y^2+z^2)^{\frac{1}{2}}.$$

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OF POOR QUALITY

Most references in the theory of elasticity deal more with two dimensional theory than that of three dimensions. Nevertheless biharmonic functions of both types show up in mathematical physics, particularly in cases involving relationships of potential, elasticity and hydromechanics. Now I will show you several groups of equations and give brief comments on each group.

MQ MODEL:
$$\sum_{j=1}^{n} d\alpha_j \, Q_j = H \tag{1}$$

$$Q_j = \left[(X - X_j)^2 + (Y - Y_j)^2 + \delta^2\right]^{1/2} \tag{2}$$

DATA EQUATIONS:
$$\sum_{j=1}^{n} d\alpha_j \, Q_{ij} = H_i \qquad i = 1,2,\ldots,n \tag{3}$$

$$Q_{ij} = \left[(X_i - X_j)^2 + (Y_i - Y_j)^2 + \delta^2\right]^{1/2} \tag{4}$$

In this group we see the original MQ method. Ordinates of H consists of linear combinations of hyperboloids centered at data points. δ was considered as a constant, whereas we will see later that it can be treated as the difference between a constant Z_j and a variable Z

MQ^{-1} MODEL:
$$G \sum_{j=1}^{n} d\alpha_j \, Q_j^{-1} = T \tag{5}$$

$$Q_j^{-1} = \left[(X - X_j)^2 + (Y - Y_j)^2 + (Z - Z_j)^2\right]^{-1/2} \tag{6}$$

DATA EQUATIONS:
$$G \sum_{j=1}^{n} d\alpha_j \, Q_{ij}^{-1} = T_i \qquad i = 1,2,\ldots,n \tag{7}$$

$$Q_{ij}^{-1} = \left[(X_i - X_j)^2 + (Y_i - Y_j)^2 + (Z_i - Z_j)^2\right]^{-1/2} \tag{8}$$

The reciprocal MQ model above is actually a point mass anomaly model for disturbing potential T. Q^{-1} is a continuous reciprocal distance function in three variables. For computational convenience we can locate point mass anomalies at a constant depth $\delta = Z_j$. We can also make all measurements of T on the XY plane at $Z = 0$. Then $(Z-Z_j)$ becomes the δ in the MQ equations of the previous group

SOLUTIONS: $$\left[d\alpha_j\right] = \left[Q_{ij}\right]^{-1}\left[H_i\right] \tag{9}$$

$$\left[d\alpha_j\right] = G\left[Q_{ij}^{-1}\right]^{-1}\left[T_i\right] \tag{10}$$

PREDICTIONS: $$\left[Q_{pj}\right]\left[Q_{ij}\right]^{-1}\left[H_i\right] = \left[\tilde{H}_p\right] \tag{11}$$

$$G\left[Q_{pj}^{-1}\right]\left[Q_{ij}^{-1}\right]^{-1}\left[T_i\right] = \left[\tilde{T}_p\right] \tag{12}$$

The solutions and predictions for MQ and reciprocal MQ, as above, follow the same basic pattern in each case. We don't need to consider these details now since this is not the main purpose of this paper.

LET $$\delta^2 = (Z - Z_j)^2 \tag{13}$$

THEN $$Q_j = \left[(X - X_j)^2 + (Y - Y_j)^2 + (Z - Z_j)^2\right]^{1/2} \tag{14}$$

The equivalence previously mentioned and identified above, causes the MQ basis function to be a Cartesian distance function in three variables, analogous to the reciprocal distance in three variables. The implication is present then, that the undetermined coefficients $d\alpha_j$ in the two cases should have the same physical meaning. This is verified by the mathematical theory of elasticity.

MQ MODEL (BIHARMONIC)

$$\nabla^2(\nabla^2 Q) = \nabla^4 Q = \frac{\partial^4 Q}{\partial X^4} + \frac{\partial^4 Q}{\partial Y^4} + \frac{\partial^4 Q}{\partial Z^4} + \frac{2\partial^4 Q}{\partial X^2 \partial Y^2} + \frac{2\partial^4 Q}{\partial Y^2 \partial Z^2} + \frac{2\partial^4 Q}{\partial Z^2 \partial X^2} = 0 \tag{15}$$

$$\nabla^4\left(\sum_{j=1}^{n} d\alpha_j Q_j\right) = 0 \tag{16}$$

Any single Q or distance function as above satisfies the biharmonic differential equation in three variables as given. Thus a linear combination of all distance functions used in MQ approximation is biharmonic.

MQ^{-1} MODEL (HARMONIC)

$$\nabla^2 (Q^{-1}) = \frac{\partial^2(Q^{-1})}{\partial X^2} + \frac{\partial^2(Q^{-1})}{\partial Y^2} + \frac{\partial^2(Q^{-1})}{\partial Z^2} = 0 \tag{17}$$

$$\nabla^2 \left(\sum_{j=1}^{n} da_j Q_j^{-1} \right) = 0 \tag{18}$$

Q^{-1} as above, is the generating function for zonal harmonics, and through the decomposition formula, leads to complete spherical harmonics satisfying the Laplace differential equation. Thus a linear combination of reciprocal MQ functions satisfies Laplace's equation.

DUCHON'S TPS:

$$W(p) = \frac{K}{8\pi D} |p - q|^2 \log |p - q| \tag{19}$$

$$|p - q| = \left[(X_p - X_q)^2 + (Y_p - Y_q)^2 \right]^{1/2} \tag{20}$$

The basic idea of Duchon's TPS is given in equations (19) and (20) above. $W(p)$ is the deflection at the point location $(X_p Y_p)$ where a concentrated load K is applied. (X_q, Y_q) is a point located on the boundary defined as a simple support for the plate. D is the constant of structural rigidity. Then $|p-q|$ is the distance between 2 points in the same plane. Note that if we let $|p-q| = r$ then equation (19) is in the simplified form $kr^2 \log r$. Log r is the well known logarithmic potential in 2 variables.

DUCHON'S MODEL:

$$\sum_{j=1}^{n} A_j \left[(X - X_j)^2 + (Y - Y_j)^2 \right] \log \left[(X - X_j)^2 + (Y - Y_j)^2 \right]^{1/2} + a_1 X + a_2 Y + a_3 = f(X,Y) \tag{21}$$

Duchon's TPS model given above indicates that f(X,Y) is a linear combination of terms $r^2 \log r$ plus three terms that physically account for rigid body displacements. These do not affect stress or strain in a thin plate

DUCHON'S DATA EQUATIONS:

$$\sum_{j=1}^{n} A_j \left[(X_i - X_j)^2 + (Y_i - Y_j)^2\right] \log \left[(X_i - X_j)^2 + (Y_i - Y_j)^2\right]^{1/2}$$

$$+ a_1 X_i + a_2 Y_i + a_3 = f(X_i, Y_i) \qquad (i = 1,2,\ldots,n)$$

WITH CONDITIONS:

$$\sum_{j=1}^{n} A_j = 0; \quad \sum_{j=1}^{n} A_j X_j = 0; \quad \sum_{j=1}^{n} A_j Y_j = 0. \tag{22}$$

The above equations show that n measurements of stress or displacement ordinates $f(X_i, Y_i)$ are sufficient to determine n values of upper case A coefficients (concentrated loads), when 3 condition equations involving rigid body motion are included in the system of equations.

ONE FORM OF HARMONIC-BIHARMONIC RELATIONS

$$\chi = r^2 \phi + \psi \tag{23}$$

χ, BIHARMONIC; ϕ AND ψ, HARMONIC.

r, DISTANCE IN 2 OR 3 VARIABLES

This relationship given above is one of several classical statements concerning biharmonic-harmonic relations in the theory of elasticity. It is applicable to both MQ and TPS.

DUCHON'S TPS BASIS

$$\chi = r^2 \text{ LOG } r + \psi \qquad r = (X^2 + Y^2)^{1/2} \tag{24}$$

$\nabla^4 \chi = 0$ BIHARMONIC IN TWO VARIABLES

Duchon's TPS is biharmonic in two variables because it can be expressed as a combination of two harmonic functions, one of which is log r, harmonic in the two variables, multiplied by the square of r in two variables. The other function is $\psi = a_1 X + a_2 Y + a_3$, also harmonic in two variables.

HARDY'S MQ BASIS

$$\chi = r^2 (1/r) + \psi \qquad r = (X^2 + Y^2 + Z^2)^{1/2} \tag{25}$$

$\nabla^4 \chi = 0$ BIHARMONIC IN THREE VARIABLES

MQ is biharmonic in three variables because it can be expressed as a combination of two harmonic functions, one of which is MQ^{-1} in three variables, multiplied by the square of r in three variables. The other harmonic function will be discussed later.

Figure 1 illustrates the cross section of a sphere after transformation of MQ and reciprocal HQ to spherical coordinates. We assume the sphere is an idealized solid elastic body with constant density or density as a function of the radius only, except for one mass element. A mass excess of daj at a single element induces a disturbing potential of the otherwise spherical equipotential with respect to the sphere. The magnitude is greatly exaggerated to show clearly the shape of the disturbed equipotential surface. MQ^{-1} approximation as a whole consists of a linear combination of ordinates of such disturbed surfaces.

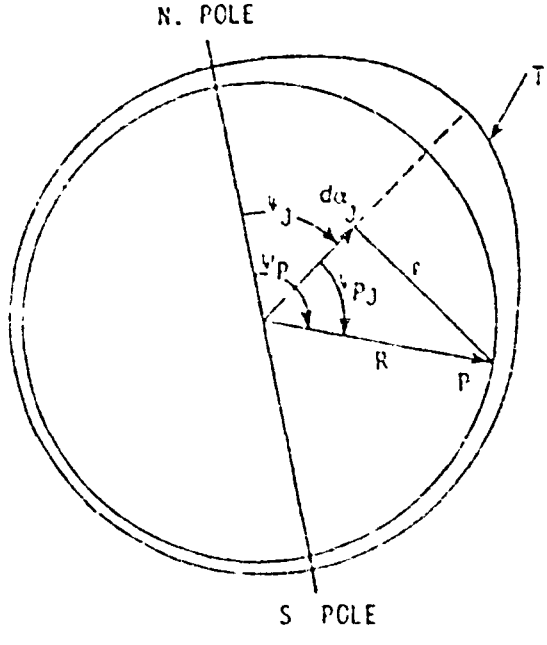

FIG 1 DISTURBING POTENTIAL

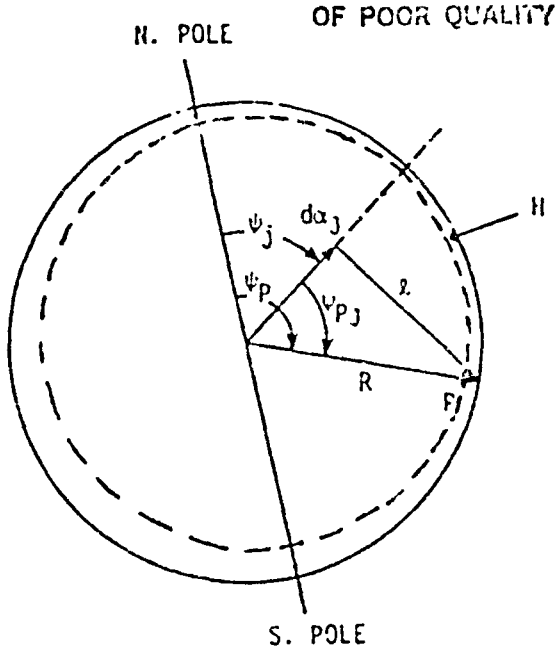

FIG. 2 BIHARMONIC DISPLACEMENT

Figure 2 is the same diagram except that it shows in exaggerated form the biharmonic displacement of the solid spherical body caused by the same point mass anomaly $d\alpha_j$. MQ approximation as a whole consists of a linear combination of ordinates of such disturbed elastic surfaces. Note that the displaced surface is inside the spherical surface for a positive anomaly, due to physical contraction of the body. The negative displacement is least nearest the anomaly and increases negatively as the spherical distance increases. An important point to be visualized with this illustration is that the point mass anomaly $d\alpha_j$ is itself displaced radially inward (for a positive anomaly) during the interaction of the standard masses and the point mass anomaly. This change in position induces a small change in the exterior disturbing potential. This induced change in the exterior harmonic function is probably associated with the form of the harmonic-biharmonic relations illustrated earlier. In brief there appears to be justification for adding three terms in one variable each because of three dimensional displacements in the solid body, and possibly a constant term as well to completely fulfill the theory of elasticity. Practically it doesn't seem necessary to include these terms when the MQ method is applied to non-elastic problems, as a general approximation scheme. I suspect the statement would be true for Duchon's TPS.

CONCLUDING REMARKS

I wish to comment briefly on a possible reason why the MQ methods gave generally better results than Duchon's TPS in Franke's study. Duchon's method involves direct application of externally concentrated forces at the surface of a reference plane; there are no body forces. The MQ methods use body forces induced by anomalous gravitation; there are no concentrated external forces. Hence the MQ biharmonic function is generally a smoother function than Duchon's TPS. This may account for some differences in the approximation properties of the two methods.

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D6

BSPLASH: A Three-Stage Surface Interpolant to Scattered Data

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ABSTRACT

Given N distinct points (x_i, y_i) and N real numbers z_i, BSPLASH constructs a function G (x, y) that satisfies $G(x_i, y_i) = z_i$ for i = 1,..., N. This C^2 interpolant consists of a bicubic spline approximation and Shepard's bivariate interpolant.

1. Introduction

This paper presents a three-stage procedure that solves the following bivariate interpolation problem. Given N distinct points in the plane (x_i, y_i) and N real numbers z_i, construct a function $G(x,y)$ that satisfies $G(x_i,y_i) = z_i$ for $i = 1,\ldots, N$. This is referred to as the scattered data interpolation problem because the data points (x_i,y_i) are not assumed to fall on a rectangular grid.

The interpolation problem can be interpreted as fitting a surface through N points in three dimensional space and thus has many applications. In mineral exploration, exploratory wells are drilled and the depths of various layers are recorded. Given this data, surfaces representing these layers can be constructed using interpolation methods. Such an example was studied by Robinson, Charlesworth, and Ellis [9] in petroleum exploration. Foley [3] and [4] used bivariate interpolation in the characterization of radio - nuclide activity resulting from nuclear tests. Samples of activity were measured at various locations, the (x_i,y_i) points, and the magnitude of the readings were the z_i's. The survey paper by Schumaker [10] gives applications in medicine, computer aided design, electronics and geology.

The new approach presented here is similar to the delta iteration methods of Foley [3] and Foley and Nielson [5], but the new method is more stable, visually smoother on smooth data, and it uses less storage. It is equally efficient on large data sets

and is capable of smoothly filling in areas that are void of data. This globally defined interpolant can be displayed by a three-dimensional surface, a contour map, or by a table of interpolated z values.

The name of the algorithm is called BSPLASH because it uses a bicubic spline approximation and a modified Shepard's interpolant. The motivation for this approach is based upon the fact that many methods that apply directly to scattered data do not yield smooth or desirable surfaces. On the other hand, many methods that yield efficient smooth interpolants only apply to data that fall on a rectangular grid.

2. Modified Shepard's Method

It will be convenient to use operator notation and to assume that there is some underlying function $f(x,y)$ defined at the data points that satisfies $f(x_i,y_i) = z_i$ for $i = 1,\ldots,N$. An easily implemented scattered data interpolant is the modified Shepard's method described in Foley [3] that is defined by

$$S[f](x,y) = \begin{cases} \dfrac{\sum_{i=1}^{N} \dfrac{f(x_i,y_i)}{p_i(x,y)}}{\sum_{i=1}^{N} \dfrac{1}{p_i(x,y)}} & \text{for } (x,y) \neq (x_j,y_j) \quad j=1,\ldots,N \\ f(x_j,y_j) & \text{for } (x,y) = (x_j,y_j). \end{cases}$$

where $d_i = (x - x_i)^2 + (y - y_i)^2$, R_i is the distance squared from (x_i, y_i) to its 5th nearest data point divided by four, and

$$p_i(x,y) = \frac{d_i(R_i + d_i)}{}.$$

This method produces an interpolant based on the inverse of the distance from a point to the data points. The proof of the following theorem can be found in Foley [6] and in Gordon and Wixom [7].

Theorem 1

Given N distinct points (x_i,y_i), then

a) S is a linear operator;

b) $S[f](x_i,y_i) = f(x_i,y_i)$ for $i = 1,\ldots,N$;

c) $S[f] \in C^{\infty}(R^2)$, that is S[f] has continuous partial derivatives of all orders for all (x,y);

d) $\frac{\partial}{\partial x} S[f](x_i,y_i) = 0$ and $\frac{\partial}{\partial y} S[f](x_i,y_i) = 0$ for $i = 1,\ldots,N$;

e) S[f] satisfies the max-min principle $\min_{i\le N} f(x_i,y_i) \le S[f](x,y) \le \max_{i\le N} f(x_i,y_i)$ for all (x,y); and

f) S[f] is invariant under translations, rotations, and magnifications of the data points (x_i,y_i).

Properties a), b), and c) state that S[f] solves the scattered data problem with a continuous function, while d) says that S[f] is flat at the data points. Property e) is important when dealing with data that has a large variation in z_i in small regions. S[f] will not oscillate violently as some other methods might. The final property implies that S[f] depends on the relative distances between data points, and not on the placement of the axes, nor on whether distances are measured in inches or miles.

Modified Shepard's interpolant is very fast computationally, requires very little storage, and easily generalizes to higher dimensions. Unfortunately, even though $S[f] \in C^{\infty}$ the plots are not visually smooth.

Figure 1 displays the plot of the bivariate function

$$(1)\quad f(x,y) = .75\exp\left(-\frac{(9x-2)^2+(9y-2)^2}{4}\right) + .75\exp\left(-\frac{(9x+1)^2}{49} - \frac{9y+1}{10}\right)$$

$$+ .5\exp\left(-\frac{(9x-7)^2+(9y-3)^2}{4}\right) - .2\exp(-(9x-4)^2 - (9y-7)^2),$$

on the domain $0 \le x \le 1$ and $0 \le y \le 1$.

From this surface, 100 data points were chosen whose (x,y) coordinates are shown in Figure 2. Each point was chosen randomly from a uniform distribution on a square with side length 1/9 centered at (i/9,j/9), i,j = 0,1,2,...,9. This function and data are used here because Franke [6] used them as his primary test case in comparing many bivariate interpolants.

Figure 3 shows the modified Shepard's interpolant applied to this data. The maximum absolute error is .2408 and the average absolute error is .0284. These errors were computed using the differences at the 33 by 33 grid used to plot the surfaces. The z_i values range from .027 to 1.17.

3. Bicubic Splines

Another major component of BSPLASH is the bicubic spline that solves the following gridded data interpolation problem. Given (XG_i, YG_j, ZG_{ij}), i = 1,...NXG and j = 1,...NYG, construct a function H(x,y) that satisfies $H(XG_i,YG_j) = ZG_{ij}$. The corresponding operator notations assumes that there is some underlying function g(x,y) defined at the grid points that satisfies $g(XG_i,YG_j) = ZG_{ij}$.

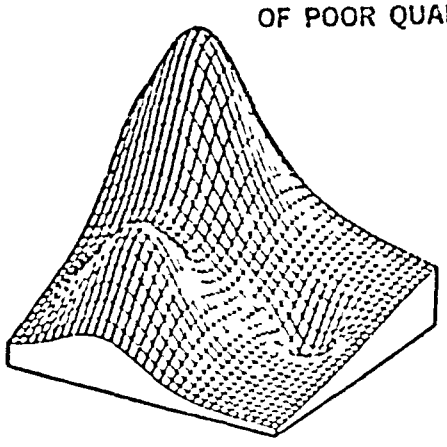


Figure 1
f(x,y)

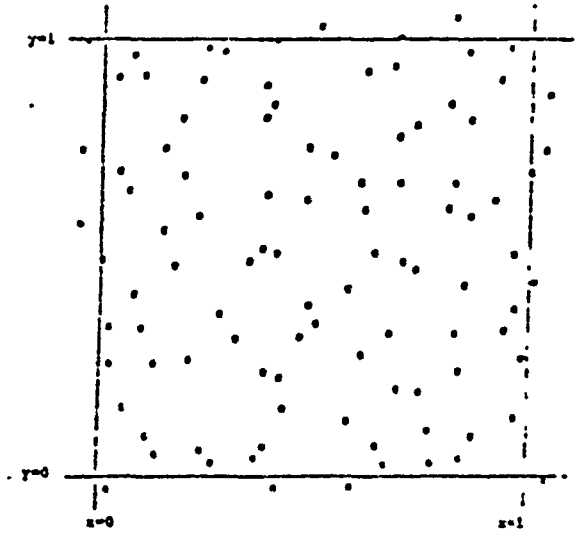


Figure 2
100 Data Points

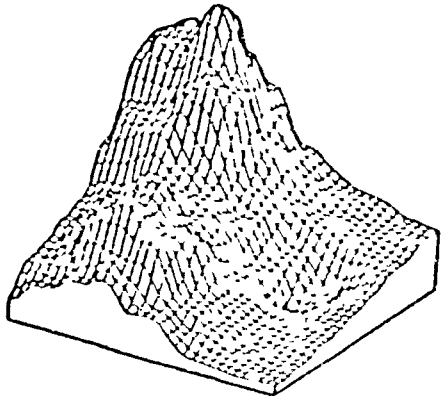


Figure 3
S(f)(x,y)

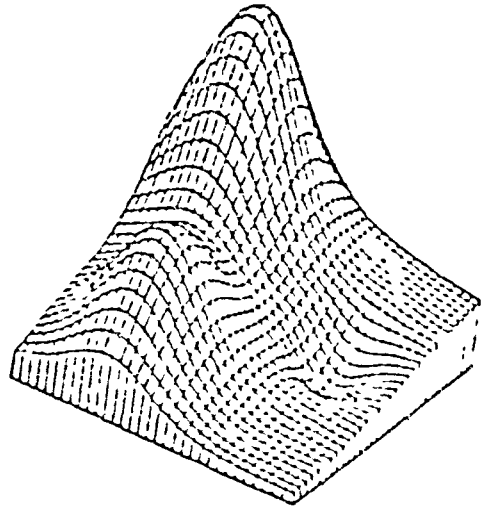


Figure 4
B(f)(x,y)

The points (XG_i, YG_j) will be referred to as the rectangular grid points.

The natural bicubic spline interpolant to g(x,y) over the grid (XG_i, YG_j) is denoted by B[g] (x,y) and it solves the gridded interpolation problem $B[g](XG_i, YG_j) = g(XG_i, YG_j)$ for i = 1,...,NXG and j = 1,...,NYG.

B[g] is formed by the tensor product of natural cubic splines in the x and y directions. The function is a piecewise bicubic polynomial of the form

$$\sum_{i=0}^{3} \sum_{j=0}^{3} b_{ij} x^i y^j$$

on each rectangle determined by the rectangular grid points (XG_i, YG_j). It is pieced together smoothly so that B[g] has all of its second order partial derivatives continuous. B[g] also minimizes the curvature functional:

$$L(f) = \iint (f_{2,2}(x,y))^2 \, dx \, dy$$

over all functions f(x,y) that solve the same gridded interpolation problem and satisfies certain continuity conditions. See deBoor [1] for a detailed description.

Other bicubic spline interpolants exist that use different end conditions. The natural end conditions were used here primarily because they were easily accessible in the software package I.M.S.L.[8] in the subroutine IBCIEU. This subroutine was applied to the test function (1) using an equally spaced 9 by 9 grid on the unit square

and this is shown in Figure 3. The maximum absolute error is .0406 and the average absolute error is .0033.

In many cases, this interpolant is a good choice for gridded data because it is computationally efficient, visually smooth, it belongs to C^2, it is globally defined, and it is easily accessible. Unfortunately, it only applies to gridded data.

4. BSPLASH

BSPLASH uses a bicubic spline and modified Shepard's method in the second and third stages of the procedure. The first stage of the alogrithm is to generate a gridded data problem. This consists of defining the rectangular grid points (XG_i, YG_j) and the values $ZG_{ij} = g(XG_i, YG_j)$ using local least squares approximations. The second stage is to form the bicubic spline through these points. The final stage adds a correction term using Shepard's method to the bicubic spline so that the scattered data interpolation problem is solved.

BSPLASH allows the user to enter his own rectangular gridpoints or else it computes the grid for him. The grid algorithm is first applied to the x_i's and then to the y_i's. The objective is to compute grid points that cover the data points (x_i, y_i) proportionally to the density of the data points without having grid points too close together or too far apart, and to have all the data points fall inside the grid. There is a restriction that $NXG \leq 25$ and $NYG \leq 25$ for large data sets.

Let $M = IROUND(\sqrt{N})$, $k = IROUND(N/M)$, $NXG = M+2$ and $NYG = M+2$. Sort the x-coordinates into increasing order. Set XG_2 to the average

of the first k x-coordinates, XG_3 to the average of the next k smallest x-coordinates,..., and XG_{M+1} to the average of the k largest x-coordinates.

Let $U = (XG_{M+1} - XG_2)/(M-1)$. If the M grid points were equally spaced, then U would be the difference between two consecutive grid points. Set $XG_1 = x_1 - U$ and $XG_{NXG} = x_N + U$ so that all of the data points fall inside the grid.

While the interior grid points are being computed, consecutive grid points are compared to see if their difference is between U/2 and 3*U. If their difference is less than U/2, they are considered to be too close and they are averaged together thus reducing NXG by one. If their difference is greater than 3*U, a new grid point is inserted at their midpoint and NXG is increased by one.

The y-coordinates of the rectangular grid are defined in the same manner.

Figure 5 shows the results of applying this grid algorithm to sets of data consisting of N = 100, 33, and 25 points. The grid points are where the orthogonal lines intersect. Note that the second highest horizontal line in Figure 5b is the average of two grid lines that were too close together. All three of these (x,y) data sets were used by Franke [6] in his comparison of many bivariate interpolants.

The rest of the first stage is to define the values $ZG_{ij} = g(XG_i, YG_j)$ at the grid points. For each of the grid points (XG_i, YG_j), find the seven nearest data points (x_k, y_k). To simplify the notation, assume that the nearest data points to (XG_i, YG_j) are

$(x_1,y_1),\ldots,(x_7,y_7)$. Let $d_k = (x_k-XG_i)^2 + (y_k-YG_j)^2$, and note that $d_1 \le d_2 \le \ldots \le d_7$. A weighted least squares fit to (x_k,y_k,z_k), $k = 1,\ldots,7$, by a quadratic is formed and then it is evaluated at (XG_i,YG_j). That is, solve

$$(2) \quad \min_{a_j} \sum_{k=1}^{7} \frac{1}{d_k} \left(g(x_k,y_k) - z_k\right)^2$$

for the a_j's, where $g(x,y) = a_1 + a_2x + a_3y + a_4x^2 + a_5xy + a_6y^2$. Then define $ZG_{ij} = g(XG_i,YG_j)$.

To add stability to this process, BSPLASH sets ZMIN = min $(z_1,\ldots,z_7)$, ZMAX = max $(z_1,\ldots,z_7)$, and then defines the grid values by

$$ZG_{ij} = \begin{cases} ZMIN & \text{if } g(XG_i,YG_j) < ZMIN \\ ZMAX & \text{if } g(XG_i,YG_j) > ZMAX \\ g(XG_i,YG_j) & \text{otherwise} \end{cases}$$

The I.M.S.L. subroutine LLSQF is used to compute $a_1,a_2,\ldots a_6$ for each of the grid points. This subroutine will properly handle the case where the minimization problem (2) has many solutions by using the fit of lowest degree.

This first stage can be used to define function values at any point, but since this depends on the seven nearest data points, the function may not be continuous. However, this weighted least squares approach gives a good local approximation to $f(x,y)$ at the rectangular grid points.

The second stage is to form the bicubic spline B[g], where $g(XG_i, YG_j) = ZG_{ij}$, $i = 1,\ldots, NXG$, and $j = 1,\ldots,NYG$. Although this generally yields a smooth approximation to f(x,y), it does not interpolate the scattered data (x_i,y_i,z_i).

The third and final stage solves the scattered data problem by adding the correction term S[f - B[g]] to B[g] to yield the BSPLASH interpolant.

$P[f](x,y) = S[f - B[g]](x,y) + B[g](x,y)$. The correction term uses the modified Shepard's method to interpolate the differences between z_i and the bicubic spline B[g] evaluated at (x_i,y_i), $i = 1,\ldots,N$.

Theorem 2

Given N distinct points (x_i,y_i) and N real numbers $z_i = f(x_i,y_i)$, then

a) P[f] solves the scattered data problem $P[f](x_i,y_i) = f(x_i,y_i)$ for $i = 1,\ldots,N$; and

b) P[f] has all of its second order partial derivatives continuous for all (x,y).

Proof:

By b) of Theorem 1, it follows that $P[f](x_i,y_i)$

$= S[f - B[g]](x_i,y_i) + B[g](x_i,y_i)$

$= f(x_i,y_i) - B[g](x_i,y_i) + B[g](x_i,y_i)$

$= f(x_i,y_i)$.

Since P[f] is the sum of C^∞ Shepard's correction function and the C^2 bicubic spline, it follows that P[f] belongs to C^2 for all (x,y).

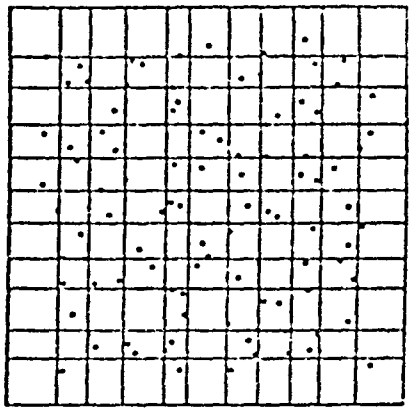
Q.E.D.

Figure 6 shows the results of BSPLASH applied to the data sets of N = 100, 33, and 25 points from (1) evaluated at the (x,y) points shown in Figure 5. The maximum absolute errors are .0443, .2293, and .1220 respectively, and the average absolute errors are .0060, .0435, and .0277 respectively.

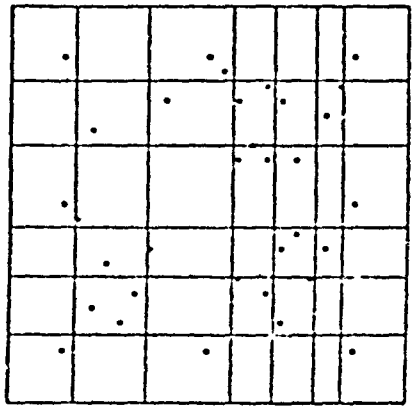
These discrete errors compare favorably with the best of the methods tested by Franke [6]. The visual smoothness of BSPLASH would also rank high with those methods. BSPLASH was applied to three other test function of Franke [6] on the same three data sets of 100, 33, and 25 points, and the results were accurate and visually smooth.

The storage required for BSPLASH is very low. Besides the storage of the data points (x_i,y_i,z_i), $i = 1,\ldots,N$, less than 3N locations are needed to store the grid, the grid's z-values, and the local parameters r_i used in modified Shepard's method. Most triangular based interpolants require storage on the order of 30N and some others require storage of more than N^2 elements.

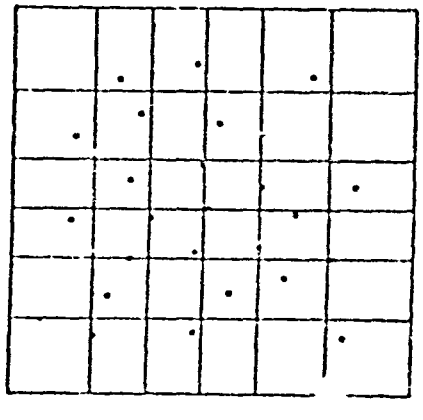
The execution times can't be accurately compared because different computers were used. The results here were done on a Cyber CDC 170/730. The overall computation time is on the order of N^2, but the observed times appear linear in N even when the grid algorithm was used. The execution times for BSPLASH when N = 25,50,100, 200, 400, and 800 points were used were 4.5, 8.3, 17.2, 39.6, 104.5, and 206.2 seconds respectively. Some other bivariate interpolants are on the order of N^3 and are not efficient for large N.



a) 100 Data Points

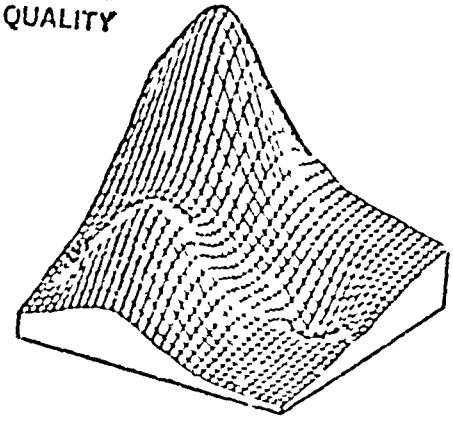


b) 33 Data Points

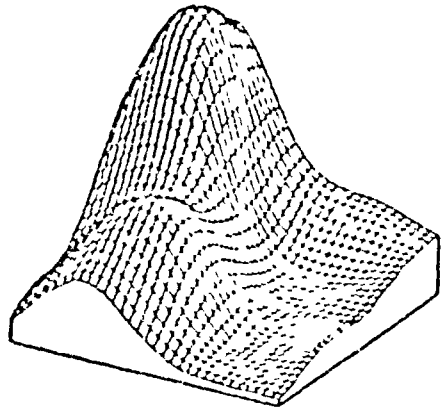


c) 25 Data Points

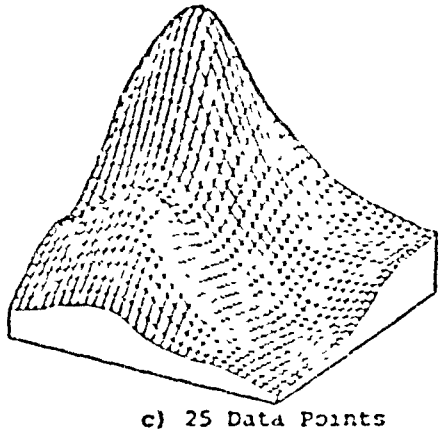
Figure 5
Data and Grid Points



a) 100 Data Points



b) 33 Data Points



c) 25 Data Points

Figure 6
BSPLAST Applied to f(x,y)

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APPENDIX

BSPLASH on Franke's Test Data

BSPLASH was applied to several sets of data that Franke[6] used in the comparison of many bivariate interpolants. Section 1 describes the data sets, ~~section 2 gives the discrete errors for BSPLASH on these~~ ~~sets~~, section 3 contains the plots of the 3-D surfaces, and section 4 lists the discrete errors of the better methods tested by Franke. The first and fourth sections are edited xeroxes of Franke's technical report.

1.2.2. The Test Problems

The basic set of test problems consisted of six different test functions over three different x-y point sets, and two x-y-z point sets from the literature, one of those used in a second version with one of the coordinates scaled. Another interesting test was the computation of a "cardinal" function obtained by setting all function values on a point set to zero, save one.

The six test functions were all to be approximated on $[0, 1]^2$. Four of them were basically obtained from McLain's paper [39], but were translated to $[0, 1]^2$ from $[1, 10]^2$ and some modified slightly to enhance the visual aspects of the surface. The other two were generated by the author to provide a fundamentally different shape in one case (saddle), and to provide a surface with a variety of behavior on one surface to serve as a principal test function.

The principal test function is given by

$$f_1(x, y) = .75 \exp\left[- \frac{(9x-2)^2 + (9y-2)^2}{4}\right] + .75 \exp\left[- \frac{(9x+1)^2}{49} - \frac{9y+1}{10}\right]$$

$$+ .5 \exp\left[- \frac{(9x-7)^2 + (9y-3)^2}{4}\right] - .2 \exp\left[- (9x-4)^2 - (9y-7)^2\right].$$

This surface consists of two Gaussian peaks and a sharper Gaussian dip superimposed on a surface sloping toward the first quadrant. The latter was included mainly to enhance the visual aspects of the surface, which is shown in Figure 4.0.1.0.

The second test function, essentially obtained from McLain is

$$f_2(x, y) = \frac{1}{9}[\tanh(9y - 9x) + 1].$$

This surface consists of two nearly flat regions of height 0 and $\frac{2}{9}$, joined

by a sharp rise, almost a cliff, running diagonally from (0, 0) to (1, 1). The test surface is shown in Figure 4.0.2.0.

The third test function was generated by the investigator and is

$$f_3(x, y) = \frac{1.25 + \cos(5.4y)}{6[1 + (3x - 1)^2]}.$$

This surface is saddle shaped and is shown in Figure 4.0.3.0.

The fourth test function, essentially obtained from McLain, is

$$f_4(x, y) = \frac{1}{3} \exp[- \frac{81}{16}((x-\frac{1}{2})^2 + (y-\frac{1}{2})^2)].$$

This surface is a Gaussian hill which slopes off in rather gentle fashion in $[0, 1]^2$. It can be seen in Figure 4.0.4.0.

The fifth test function was also essentially obtained from McLain and is

$$f_5(x, y) = \frac{1}{3} \exp[- \frac{81}{4}((x-\frac{1}{2})^2 + (y-\frac{1}{2})^2)].$$

This surface is a steep Gaussian hill which becomes almost zero at the boundaries of the unit square. It can be seen in Figure 4.0.5.0.

The sixth test function is also essentially from McLain, and is

$$f_6(x, y) = \frac{1}{9}[64 - 81((x-\frac{1}{2})^2 + (y-\frac{1}{2})^2)]^{\frac{1}{2}} - \frac{1}{2}.$$

This surface represents the part of a sphere above the unit square. The sphere is of radius $\frac{8}{9}$ with center at $(\frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$. The surface is shown in Figure 4.0.6.0.

There were three different sets of points over $[0, 1]^2$ used in the tests. The first set consisted of 100 points generated by a pseudorandom number generator, one point in each square of side $\frac{1}{9}$ centered at $(\frac{i}{9}, \frac{j}{9})$ for $i, j = 1, \ldots, 10$. This yields a set of scattered points forced to have

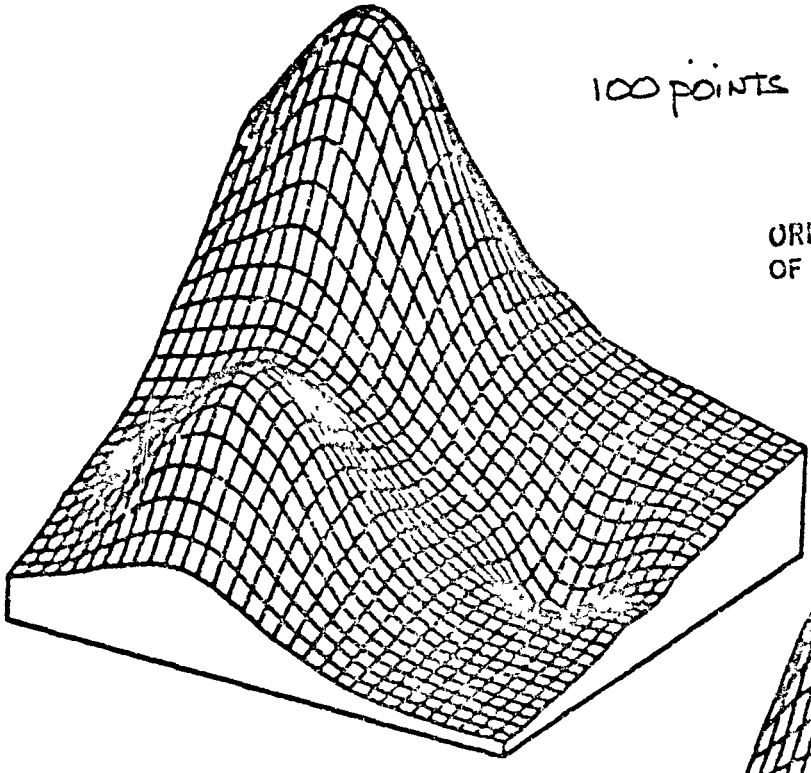
somewhat uniform density, although as can be seen in Figure 0.1.0.0. there are locally large variations in density. The triangulated set of points is also shown in Figure 0.1.0.0. Part of the unit square is outside of the convex hull. The points are listed in Table 1.

The second set of data consists of 33 points and was generated by the investigator to purposely have some areas sparsely populated by points while other areas are not. This set of points is shown in Figure 0.2.0.0. The points are listed in Table 2.

The third set of points was digitized by Gregory M. Nielson and is similar in disposition to a set of points appearing in McLain [40]. This set of points is shown in Figure 0.3.0.0. Part of the unit square is outside the convex hull. The points are listed in Table 3.

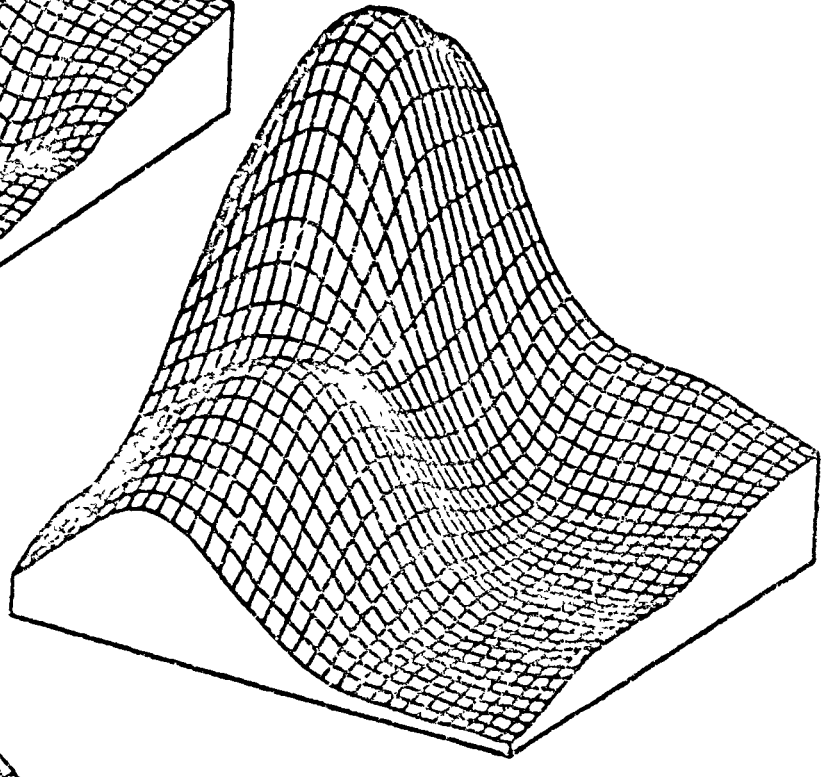
Two sets of data were obtained from the literature, and one of these was scaled in one variable to obtain another. A fourth set was used to generate a "Cardinal Function". The data given in Table 3, and shown in Figure 0.3.0.0. was given the following function values: $f(x_k, y_k) = 0$ except $f(.1875, .2625) = .2$. Here .2 was used for visual purposes rather than 1 as would ordinarily be done for a true cardinal function. This gives some information about the influence of one point on the surface for moderate sized point sets. Of the two sets of points from the literature, one is from Akima [1] and was obtained during a study of waveform distortion. It is repeated here in Table 5, and shown in Figure 0.5.0.0. The second was obtained from Ferguson [14] and is repeated here in Table 6, and shown in Figure 0.6.0.0. The same set of data, but with the y coordinate multiplied by three was also used to show effects of scaling only one variable, and is shown in Figure 0.7.0.0. For visual purposes, the function values given in Table 2 are actually .5 more than given by Ferguson. As can be seen from Figure

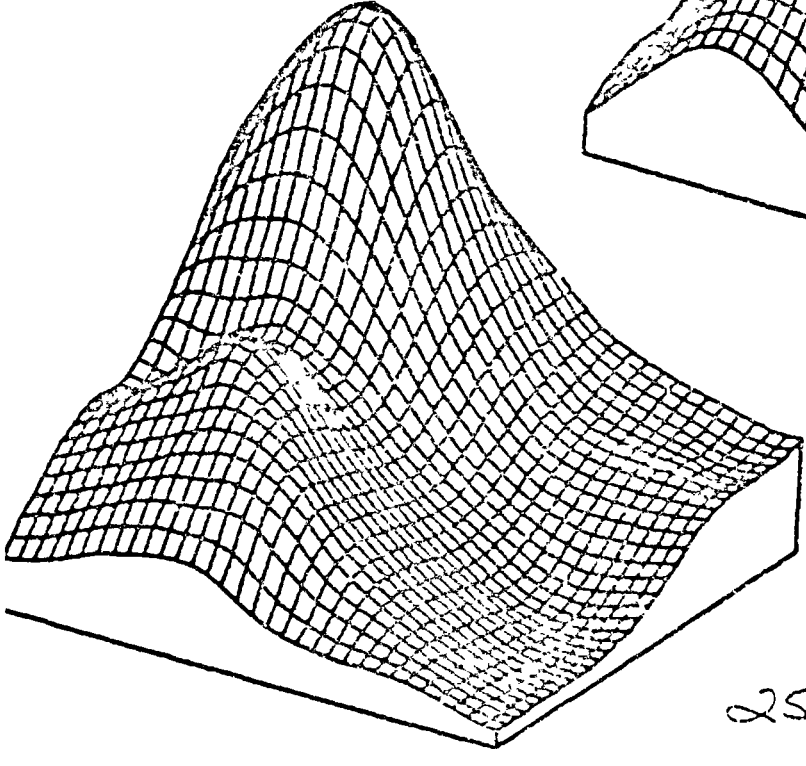
BSPLASH on F1(x,y)



100 POINTS

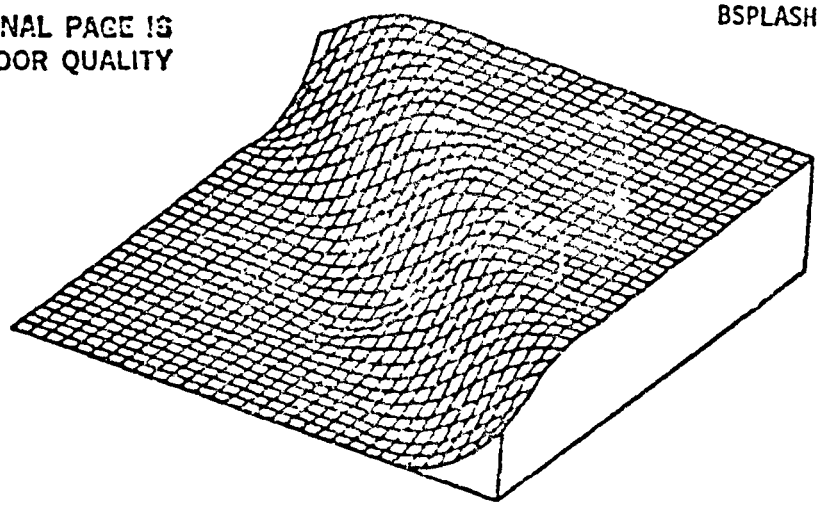
33 POINTS



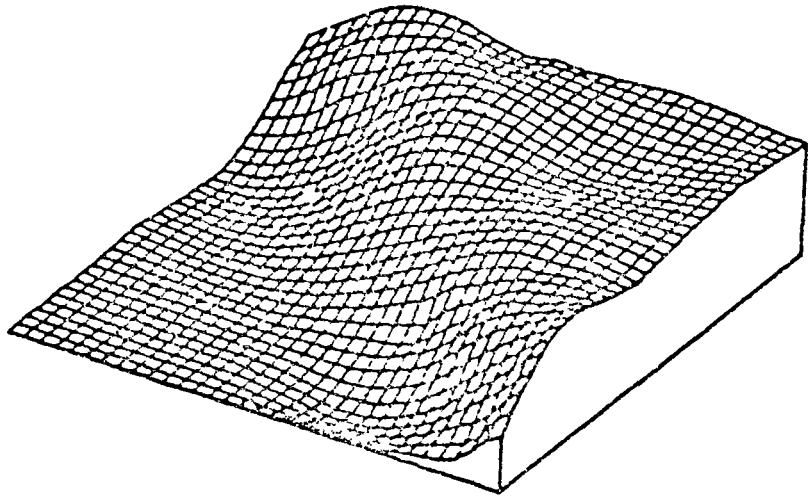


25 points

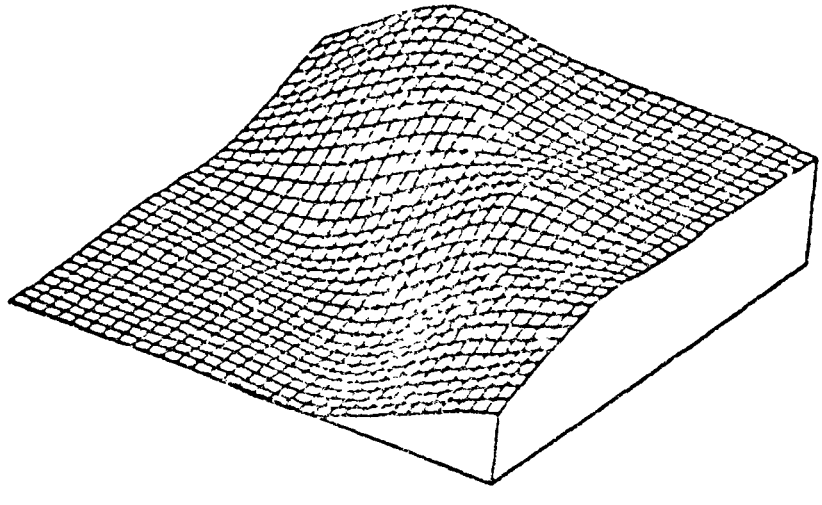
BSPLASH ON F2 (x, y)



100 points

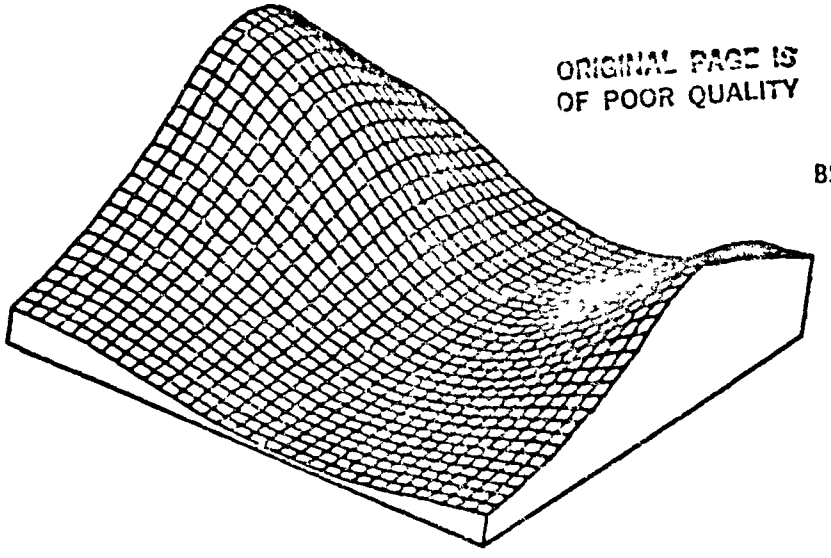


33 points

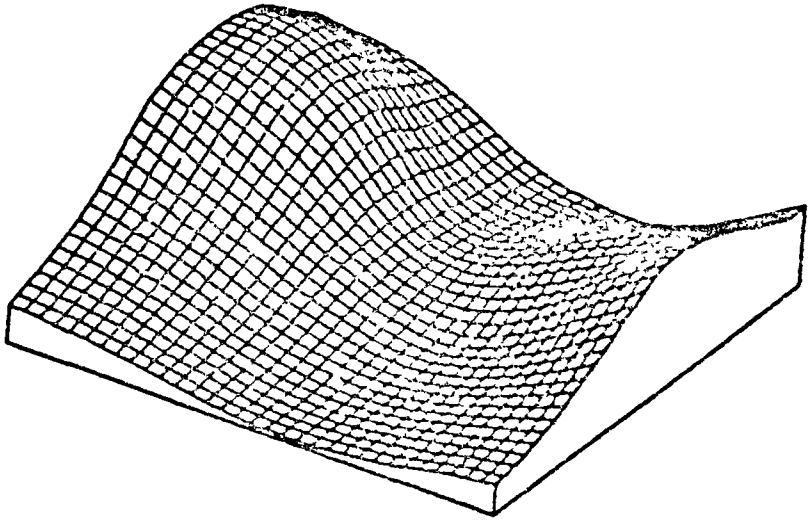


25 points

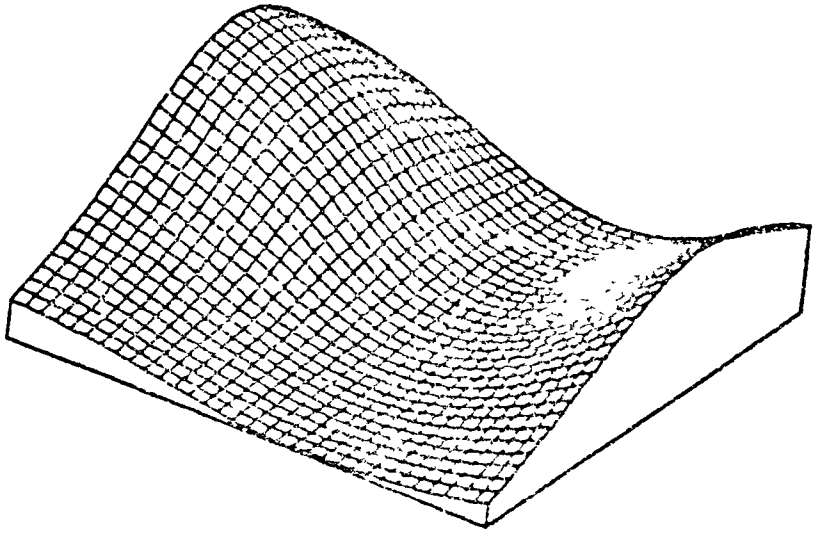
BSPLASH ON F3 (x, y)



100 points

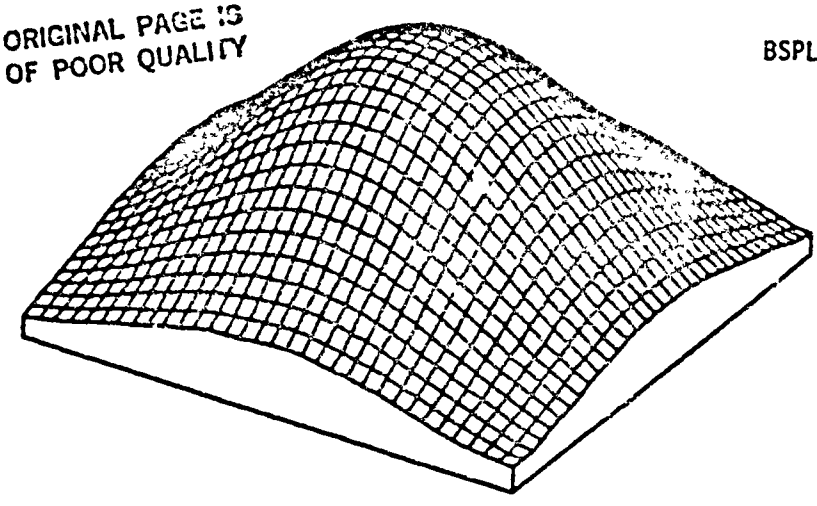


33 points

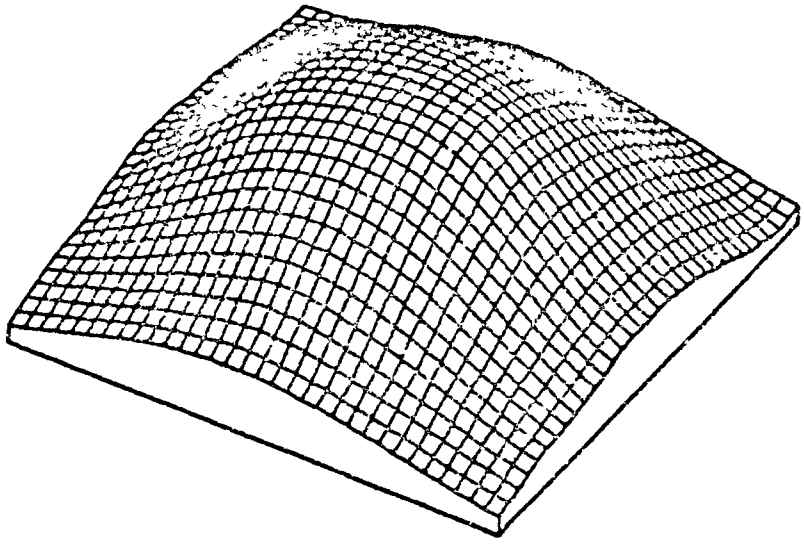


25 points

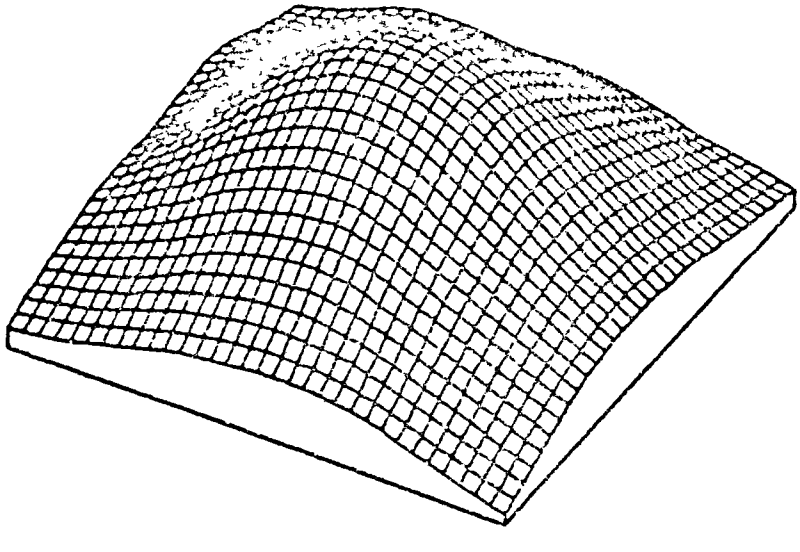
BSPLASH on F4 (x, y)



100 Points

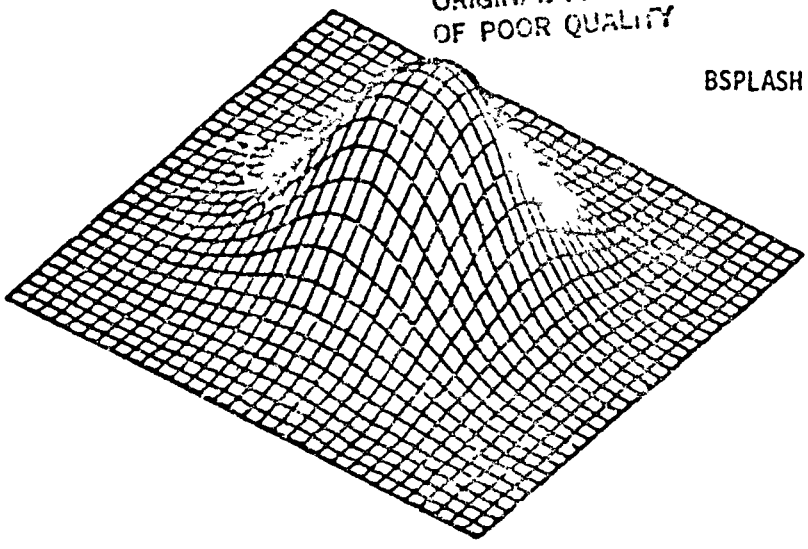


33 points

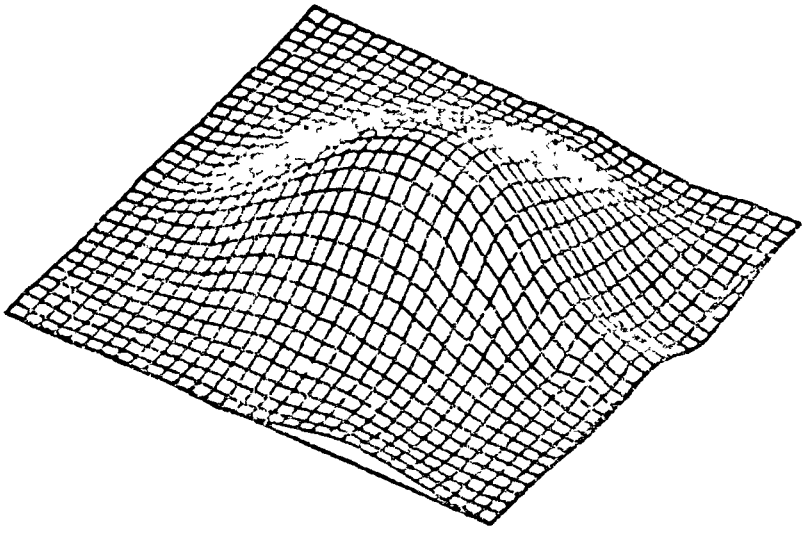


25 points

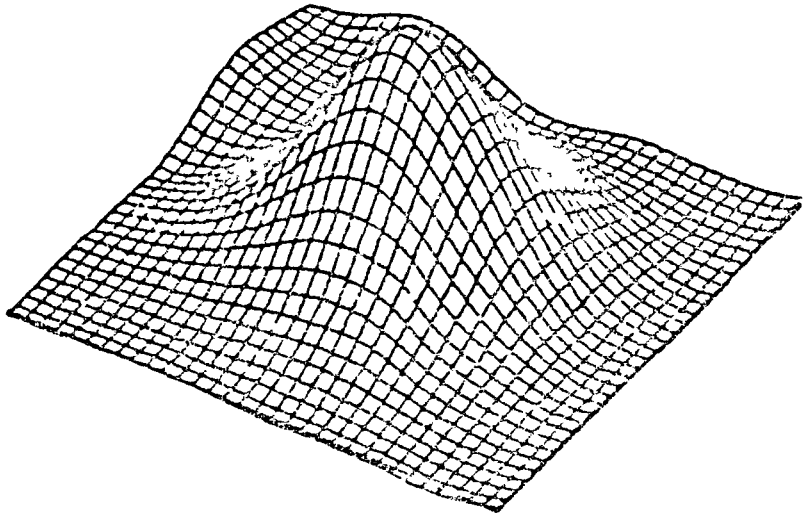
BSPLASH on F5 (x, y)



100 points

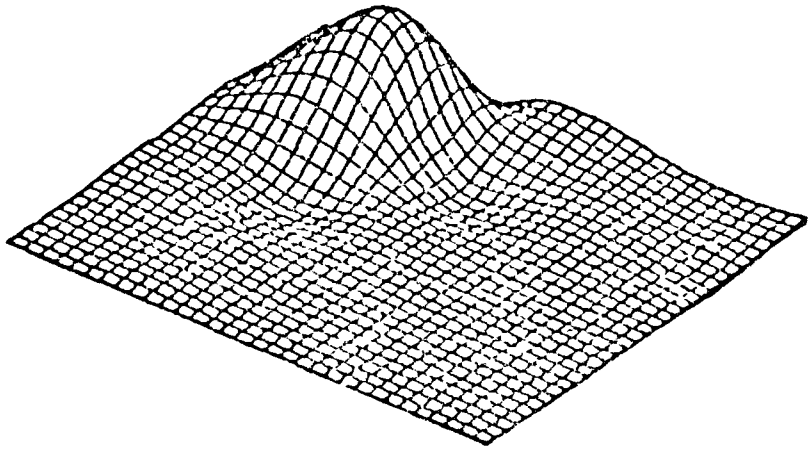


33 points



25 points

AKIMA'S DATA
FERGUSON'S DATA



25 point "Cardinal"

Method F1, 100 pts	Maximum Deviation	Mean Deviation	RMS Deviation
1: Franke - 3	.0919	.00812	.0148
4: Akima	.0647	.00787	.0125
10: Akima Mod. I	.0856	.00784	.0133
13: Nielson - Franke Q	.0782	.00741	.0122
14: Mod. Quad. Shepard	.0573	.00785	.0128
16: Akima Mod. III	.0520	.00729	.0117
24: Franke - TPS	.0940	.00887	.0164
28: Lawson	.0951	.00783	.0124
19: Nielson MinNorm	.0492	.00537	.00940
21: Hardy Quadric	.0225	.00181	.00357
23: Duchon TPS	.0518	.00525	.00947
27: Hardy Recip. Quad.	.0247	.00283	.00518
30: Foley III	.0636	.00473	.00941
BSPLASH	.0443	.0060	

Method F_1 33 pts	Maximum Deviation	Mean Deviation	RMS Deviation
1: Franke - 3	.347	.0477	.0732
4: Akima	.158	.0384	.0535
10: Akima Mod I	.197	.0400	.0570
13: Nielson - Franke Q	.150	.0326	.0455
14: Mod Quad. Shepard	.184	.0340	.0476
16: Akima Mod. III	.164	.0372	.0521
24: Franke - TPS	.218	.0346	.0517
28. Lawson	.287	.0462	.0657
19: Nielson MinNorm	.150	.0305	.0437
21: Hardy Quadric	.137	.0181	.0269
23: Duchon - TPS	.153	.0293	.0421
27: Hardy Recip. Quad.	.140	.0153	.0244
30: Foley III	.296	.0350	.0546
BSPLASH	.229	.0435	

Method F_1 25 pts	Maximum Deviation	Mean Deviation	RMS Deviation
1: Franke - 3	.240	.0359	.0486
4: Akima	.134	.0282	.0386
10: Akima Mod. I	.129	.0280	.0380
13: Nielson - Franke Q	.153	.0350	.0478
14: Mod. Quad Shepard	.158	.0353	.0486
16. Akima Mod III	.155	.0355	.0484
24: Franke - TPS	.129	.0267	.0374
28: Lawson	.202	.0327	.0458
19. Nielson MinNorm	.124	.0235	.0323
21: Hardy Quadric	.119	.0235	.0322
23 Duchon TPS	.121	.0253	.0348
27: Hardy Recip. Quad.	.119	.0214	.0294
30: Foley III	.165	.0196	.0310
BSPLASH	.122	.0277	

		MAX	MEAN	
1:	Franke - 3	.0518	.00286	.00586
4:	Akima	.0520	.00303	.00609
10:	Akima Mod. I	.0473	.00257	.00512
13:	Nielson - Franke Q	.0721	.00265	.00683
14:	Mod. Quad. Shepard	.0468	.00264	.00551
16:	Akima Mod. III	.0958	.00293	.00809
24:	Franke - TPS	.0295	.00243	.00433
28:	Lawson	.0280	.00271	.00448
19:	Nielson MinNorm	.0424	.00181	.00434
21:	Hardy Quadric	.0244	.00177	.00333
23:	Duchon - TPS	.0344	.00210	.00436
27:	Hardy Recip. Quad.	.0379	.00192	.00338
30:	Foley III	.0281	.00223	.00419
	BSPLASH	.0265	.0021	

Deviations from Cliff test surface, 100 points

Table D.1.2

F2

1:	Franke - 3	.0776	.0124	.0190
4:	Akima	.0543	.00850	.0133
10:	Akima Mod. I	.0513	.00747	.0122
13:	Nielson - Franke Q	.0878	.0137	.0219
14:	Mod. Quad. Shepard	.0876	.0121	.0206
16:	Akima Mod. III	.0680	.0106	.0176
24:	Franke - TPS	.0561	.00913	.0147
28:	Lawson	.0956	.0126	.0205
19:	Nielson MinNorm	.0582	.00800	.0140
21:	Hardy Quadric	.0577	.0129	.0170
23:	Duchon - TPS	.0526	.00777	.0134
27:	Hardy Recip. Quad.	.0500	.00853	.0130
30:	Foley III	.0914	.0165	.0262
	BSPLASH	.0493	.0090	

Deviations from Cliff test surface, 33 points

Table D.2.2

F2

1:	Franke - 3	.101	.0225	.0408
4:	Akima	.0999	.0148	.0257
10:	Akima Mod. I	.0987	.0143	.0252
13:	Nielson - Franke Q	.148	.0166	.0304
14:	Mod. Quad. Shepard	.163	.0166	.0314
16:	Akima Mod. III	.146	.0164	.0305
24:	Franke - TPS	.106	.0148	.0257
28:	Lawson	.132	.0164	.0283
19:	Nielson MinNorm	.0942	.0138	.0242
21:	Hardy Quadric	.0995	.0143	.0231
23:	Duchon - TPS	.101	.0135	.0235
27:	Hardy Recip. Quad	.105	.0139	.0236
30:	Foley III	.0932	.0165	.0250
	BSPLASH	.0779	.0107	

Deviations from Cliff test surface, 25 points

F2

		MAX.	MEAN	
1:	Franke - 3	.0198	.00164	.00294
4:	Akima	.0274	.00224	.00423
10:	Akima Mod. I	.0254	.00198	.00367
13:	Nielson - Franke Q	.0168	.00110	.00206
14:	Mod. Quad. Shepard	.0125	.00112	.00194
16:	Akima Mod. III	.0142	.00105	.00202
24:	Franke - TPS	.0165	.00157	.00273
28:	Lawson	.0565	.00149	.00359
19:	Nielson MinNorm	.0195	.00091	.00200
21:	Hardy Quadric	.00461	.00025	.00052
23:	Duchon - TPS	.00597	.00049	.00092
27:	Hardy Recip. Quad.	.00928	.00068	.00136
30:	Foley III	.0117	.00117	.00196
	BSPLASH	.0195	.0010	

Deviations from Saddle test surface, 100 points

Table D.1.3

1:	Franke - 3	.111	.0121	.0224
4:	Akima	.0578	.0110	.0165
10:	Akima Mod. I	.0578	.0104	.0156
13:	Nielson - Franke Q	.0679	.00939	.0146
14:	Mod. Quad. Shepard	.0724	.00907	.0139
16:	Akima Mod. III	.0597	.0104	.0162
24:	Franke - TPS	.0662	.0109	.0175
28:	Lawson	.0585	.0133	.0199
19:	Nielson MinNorm	.0571	.0102	.0159
21:	Hardy Quadric	.0262	.00442	.00689
23:	Duchon - TPS	.0574	.00912	.0140
27:	Hardy Recip. Quad.	.0505	.00571	.00970
30:	Foley III	.0885	.00888	.0148
	BSPLASH	.0723	.0105	

Deviations from Saddle test surface, 33 points

1:	Franke - 3	.0688	.0111	.0171
4:	Akima	.0861	.0121	.0202
10:	Akima Mod. I	.0866	.0119	.0203
13:	Nielson - Franke Q	.0794	.0115	.0189
14:	Mod. Quad. Shepard	.0759	.0114	.0183
16:	Akima Mod. III	.0787	.0116	.0189
24:	Franke - TPS	.0714	.00983	.0171
28:	Lawson	.0875	.0126	.0205
19:	Nielson MinNorm	.0704	.0100	.0172
21:	Hardy Quadric	.0397	.00570	.00952
23:	Duchon - TPS	.0588	.00810	.0137
27:	Hardy Recip. Quad.	.0443	.00528	.00955
30:	Foley III	.0823	.00853	.0165
	BSPLASH	.0397	.0065	

Deviations from Saddle test surface, 25 points

		MAX.	MEAN	
1:	Franke - 3	.0114	.00122	.00189
4:	Akima	.0101	.00124	.00177
10:	Akima Mod. I	.00675	.00102	.00113
13:	Nielson - Franke Q	.00517	.00058	.00083
14:	Mod. Quad. Shepard	.00388	.00065	.00089
16:	Akima Mod. III	.00230	.00049	.00070
24:	Franke - TPS	.00560	.00103	.00141
28:	Lawson	.00899	.00061	.00109
19:	Nielson MinNorm	.00303	.00047	.00069
21:	Hardy Quadric	.00102	.00005	.00011
23:	Duchon - TPS	.00294	.00017	.00030
27:	Hardy Recip. Quad.	.00227	.00034	.00050
30:	Foley III	.00604	.00083	.00117
	BSPLASH	.0077	.0006	

Deviations from Gentle test surface, 100 points F_4

Table D.1.4

1:	Franke - 3	.0446	.00608	.0101
4:	Akima	.0167	.00487	.00623
10:	Akima Mod. I	.0160	.00442	.00573
13:	Nielson - Franke Q	.0312	.00422	.00637
14:	Mod. Quad. Shepard	.0272	.00451	.00679
16:	Akima Mod. III	.0204	.00394	.00565
24:	Franke - TPS	.0339	.00681	.0107
28:	Lawson	.0269	.00552	.00815
19:	Nielson MinNorm	.0214	.00371	.00563
21:	Hardy Quadric	.00724	.00121	.00201
23:	Duchon - TPS	.0259	.00415	.00714
27:	Hardy Recip. Quad.	.0188	.00266	.00485
30:	Foley III	.0349	.00438	.00674
	BSPLASH	.0319	.0047	

Deviations from Gentle test surface, 33 points F_4

1:	Franke - 3	.0247	.00491	.00651
4:	Akima	.0256	.00541	.00716
10:	Akima Mod. I	.0248	.00541	.00681
13:	Nielson - Franke Q	.0340	.00562	.00746
14:	Mod. Quad. Shepard	.0227	.00529	.00669
16:	Akima Mod. III	.0232	.00575	.00760
24:	Franke - TPS	.0245	.00440	.00586
28:	Lawson	.0234	.00399	.00541
19:	Nielson MinNorm	.0161	.00307	.00433
21:	Hardy Quadric	.00709	.00107	.00158
23:	Duchon - TPS	.0128	.00265	.00351
27:	Hardy Recip. Quad.	.00528	.00055	.00079
30:	Foley III	.0224	.00436	.00588
	BSPLASH	.0221	.0038	

Deviations from Gentle test surface, 25 points F_4

Table D.3.4

		MAX.	MEAN	
1:	Franke - 3	.0358	.00228	.00447
4:	Akima	.0434	.00242	.00510
10:	Akima Mod. I	.0317	.00215	.00436
13:	Nielson - Franke Q	.0206	.00176	.00337
14:	Mod. Quad. Shepard	.0218	.00182	.00361
16:	Akima Mod. III	.0212	.00171	.00337
24:	Franke - TPS	.0284	.00212	.00418
28:	Lawson	.0216	.00154	.00323
19:	Nielson MinNorm	.0195	.00101	.00229
21:	Hardy Quadric	.00280	.00012	.00031
23:	Duchon - TPS	.0175	.00038	.00217
27:	Hardy Recip. Quad.	.00736	.00030	.00078
30:	Foley III	.0143	.00172	.00282
	BSPLASH	.0263	.0016	

Deviations from Steep test surface, 100 points

Table D.1.5

1:	Franke - 3	.143	.0162	.0298
4	Akima	.115	.0120	.0240
10:	Akima Mod. I	.109	.0113	.0227
13:	Nielson - Franke Q	.0835	.0104	.0181
14.	Mod. Quad. Shepard	.110	.0113	.0220
16:	Akima Mod. III	.115	.0119	.0240
24:	Franke TPS	.150	.0148	.0305
28.	Lawson	139	.0129	.0289
19	Nielson MinNorm	.115	.0105	.0228
21:	Hardy Quadric	.0716	.00850	.0148
23	Duchon - TPS	.149	.0130	.0296
27:	Hardy Recip. Quad	.0963	.00878	.0180
30	Foley III	.110	.0143	.0249
	BSPLASH	.1267	.0139	

Deviations from Steep test surface, 33 points

Table D.2.5

1.	Franke - 3	.113	.0178	.0257
4	Akima	.0534	.0103	.0149
10	Akima Mod. I	.0520	.0103	.0140
13	Nielson - Franke Q	.0550	.00850	.0127
14	Mod. Quad. Shepard	.0468	.00911	.0126
16	Akima Mod. III	.0510	.00928	.0128
24	Franke - TPS	.0317	.0079	.0100
28.	Lawson	.0455	.0129	.0235
19	Nielson MinNorm	.0314	.00987	.00664
21.	Hardy Quadric	.0189	.00453	.00695
23	Duchon - TPS	.0233	.00827	.00683
27	Hardy Recip. Quad.	.0141	.00713	.00456
30	Foley III	.0713	.0107	0161
	BSPLASH	.0402	.0066	

Deviations from Steep test surface, 25 points

Table D.3.5

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Smoothing Surfaces Using Generalized Cross Validation

by Douglas Bates

Grace Wahba
Jim Wendelburger
Finbarr O'Sullivan
Miquel Villalobis
others

Outline:

Smoothing Surfaces

Cross Validation

Generalized Cross Validation

Computational Difficulties

Applications to Classification Problems

SMOOTHING SURFACES

APPROXIMATING SURFACES

BASIS FUNCTIONS

$$\phi_i(\underline{t}) \rightarrow f(\underline{t}) = \sum_{i=1}^{N} c_i \phi_i(\underline{t})$$

N AS LARGE AS 100's
(1000's)

PENALIZE FUNCTION FOR
BENDING

$$\int_{\Omega} (Kf)^2 = \underline{c}' \not{\underline{\underline{K}}} \underline{c}$$

$\not{\underline{\underline{K}}}$ REPRESENTS A (SEMI)-NORM

BALANCE TWO CRITERIA

1) FIDELITY TO DATA

MEASURED BY

$$\sum_{j=1}^{n} \left(y_j - \sum_{i=1}^{N} c_i \phi_i(t_j) \right)^2$$

OR OTHER CRITERIA

- WEIGHTED LEAST SQUARES

2) SMOOTHNESS

MEASURED BY $\underline{c}' \underline{\underline{\Phi}} \underline{c}$

COMBINE AS

$$\min_{\underline{c} \in \mathbb{R}^n} \frac{1}{n} \| \underline{y} - \underline{\underline{X}} \underline{c} \|^2 + \lambda \underline{c}' \underline{\underline{\Phi}} \underline{c} \qquad (4)$$

$$\{X\}_{ji} = \phi_i(t_j)$$

WHAT λ ?

CROSS VALIDATION

GENERAL IDEA

USE PART OF THE DATA TO ESTIMATE f AND FIND OUT HOW WELL IT FITS THE REST

REPEAT FOR VARIOUS λ

IN PARTICULAR:

FIX λ

FOR EACH $j = 1, \ldots, N$

DELETE j'TH OBS.

PREDICT $f(t_j)$ FROM REMAINING DATA. PREDICTION IS $f_{j\lambda}^{[j]}$

CHOOSE λ TO MINIMIZE

$$\sum_{j=1}^{N} (y_j - f_{j\lambda}^{[j]})^2$$

PROBLEMS

1) MASSIVE AMOUNT OF COMPUTATION

2) OTHER DEFICIENCIES

SEE GOLUB, HEATH, & WAHBA
TECHNOMETRICS, 1978 (±1)

GENERALIZED CROSS VALIDATION

- ROTATIONALLY INVARIANT FORM OF CROSS VALIDATION

- ALSO, FOR FIXED λ

$\underline{\hat{y}}_\lambda$ LINEAR IN $\underline{y}$

IE. $\underline{\hat{y}}_\lambda = A(\lambda)\,\underline{y}$

$A(\lambda)$ IS A PROJECTION

λ CHOSEN TO MINIMIZE

$$V(\lambda) = \frac{\| (I - A(\lambda))\,\underline{y} \|^2}{[\mathrm{tr}\,(I - A(\lambda))]^2}$$

COMPUTATIONAL METHODS:

$A(\lambda)$ CAN BE EXPRESSED AS

$$X(X'X+n\lambda\Phi)^{-1}X'$$

Φ POSITIVE DEFINITE

FACTOR $\Phi = R'R$

R - UPPER TRIANGULAR

LET $\underline{\gamma} = R\underline{c}$

$$C = XR$$

(1) IS NOW $\min_{\underline{\gamma} \in R^N} \frac{1}{n}\|\underline{y} - C\underline{\gamma}\|^2 + \lambda \underline{\gamma}'\underline{\gamma}$

TAKE S.V.D. OF C AS

$$C = UDV'$$

$$U'U = I$$

$$V'V = VV' = I$$

D diagonal $(d_1, d_2, \ldots, d_N)$

$$A(\lambda) = UD(D^2 + n\lambda)^{-1} DU'$$

LET $z = U'y$

$$V(\lambda) = \frac{\sum_{j=1}^{N} \left(\frac{n\lambda}{d_j^2 + n\lambda}\right)^2 z_j^2 + \sum_{j=N+1}^{n} z_j^2}{\left(\sum_{j=1}^{N} \left(\frac{n\lambda}{d_j^2 + n\lambda}\right) + n - N\right)^2}$$

EASY TO EVALUATE

MIN USUALLY HAS $n\lambda$ WITHIN $d_1^2, d_2^2, \ldots, d_{50}^2$ OR SO

DIFFICULTY

REQUIRES S.V.d. OF LARGE (USUALLY ILL-CONDITIONED) MATRIX C

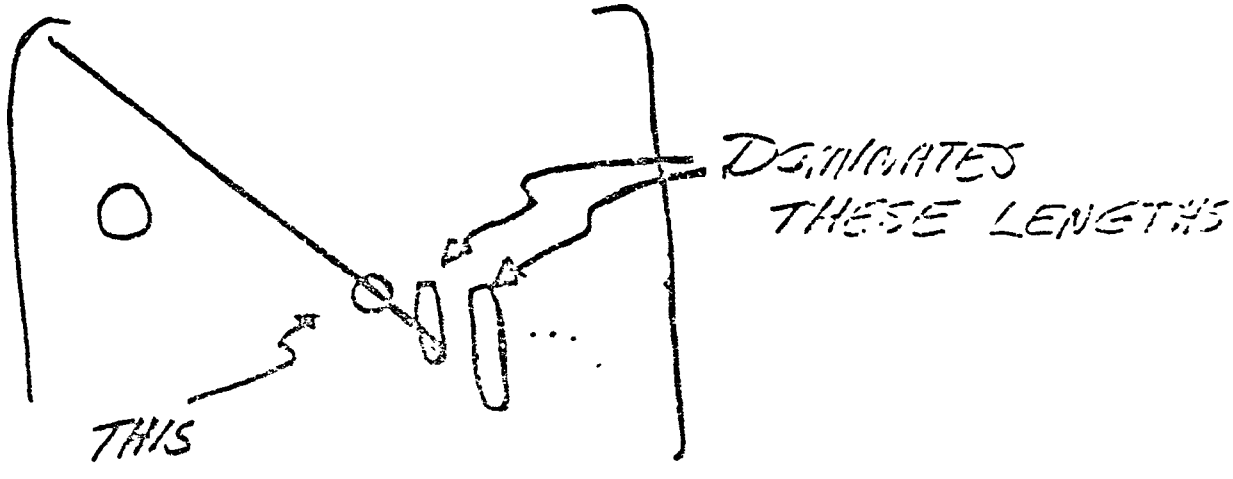
CAN GET LARGE SING. VALUES (& LEFT VECTORS) WITH A PIVOTED QR DECOMP. FIRST.

$CE = QR$

E - PERMUTATION

Q - ORTHOGONAL

R - UPPER TRIANGULAR
- DECREASING DIAGONALS



CUT OFF R AT k ROWS WHERE k CHOSEN SO $(R_k^* R_k - C^* C)$ SMALL

POSITIVE SEMI-DEFINITES

SIMILAR FORMULATION BUT USE A PIVOTED CHOLESKY DECOMPOSITION OF Σ

Classification Applications

$\underline{t}$ multivariate observations

2 populations (can be >2)

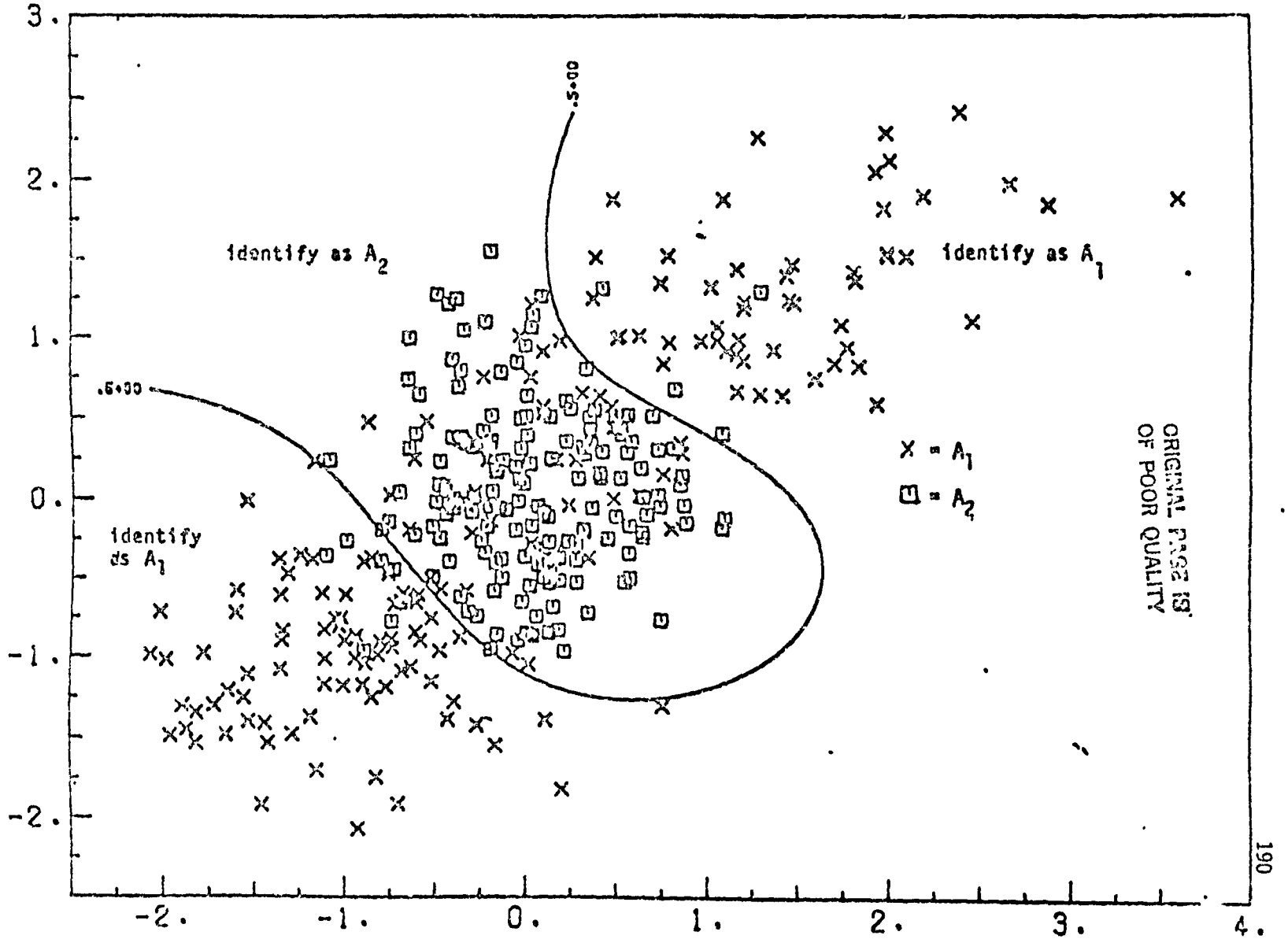
training samples from populations 1 & 2

Set $Y_i = 1$ for each $\underline{t}_i$ in population 1
$Y_i = 0$ for each $\underline{t}_i$ in population 2

Like noisy data generated by real valued fundtion in R^k

Function is relative likelihood of sample 1 at that point.

Fit surface using Cross Validated Multivariate Thin Plate Splines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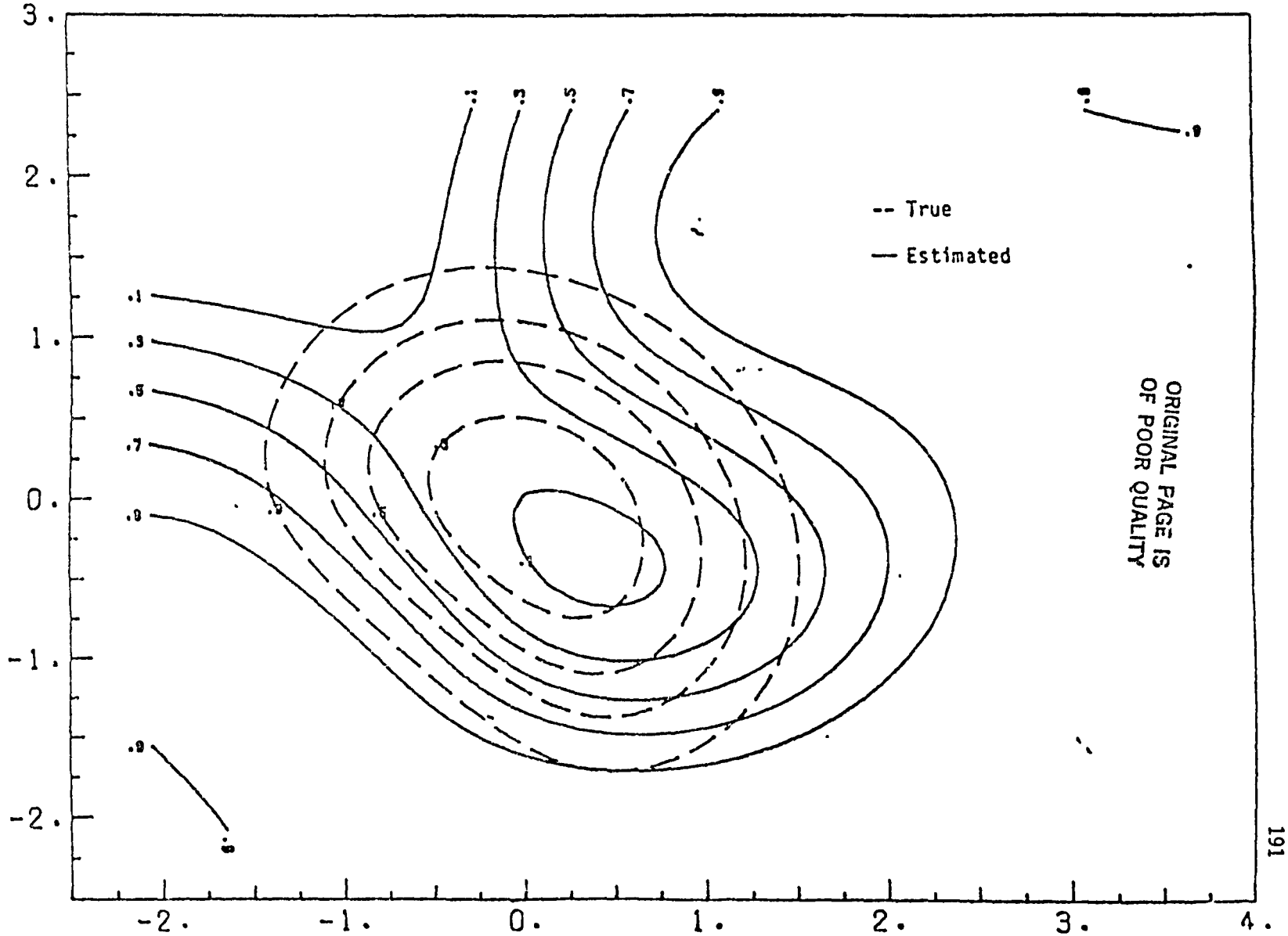
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Applications of Surface Modelling Techniques to Engineering Problems

Rosemary E. Chang

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THE UNIVERSITY OF UTAH

DEPARTMENT OF MATHEMATICS
SALT LAKE CITY UTAH 84112
801 581-6851

May 20, 1982

Professor Larry L. Schumaker
Department of Mathematics
Texas A & M University
College Station, TX 77843

Dear Larry:

Thank you for your kind attentions at the NASA Workshop on Surface Fitting. You and your colleagues did a nice job of making us all feel at home. I regretted missing the panel discussion (and the party!). Perhaps you can let me know some of what was said.

I have been thinking about what might be useful to NASA on Surface Fitting. The only talk that really was on NASA problems was Heydorn's talk, which focused on statistical methods. I happen to have had a slight exposure to LANDSAT data from some University of Utah geographers. The surface methods customarily used seemed to be piecewise linear or piecewise bilinear, which is a bit naive. Heydorn's talk contained an interesting picture of fields of wheat, corn, or "idle". This screamed for Little's arbitrary quadrilateral patches and/or Gregory and Charrot's putting triangular patches into a system of rectangular patches.

A rendering issue. I was surprised that NASA thinks it can understand surfaces from flat pictures. I think that interactive graphics rendering is the absolutely bare minimum for having the illusion of understanding 3D surfaces. A milled model is better. Some of these points were made in the DoE article by Barnhill and Chang which Chang referenced. This document might have some utility toward NASA applications - let me know if you have a copy or not.

For arbitrarily spaced data when there is a lot of data, I think that adaptive methods, such as in Vittitow's PhD. thesis at Utah, are a good idea.

In conclusion, I have the following broadly-based thoughts:

1. The richness of possibilities for surface representation: The most important thing about surfaces is to get one. Operation counts and all that pale in comparison to getting *some* solution to the problem at hand. Once *a* solution is found, it becomes rather routine to improve it.

2. Multidimensional problems 3D and 4D surfaces are what have research significance. Curves have been over-studied, even though there remain unanswered questions, e.g., parametrization. But just to say "3D surface" is insufficient. One must tailor the surface to the problem at hand.

3. What can NASA do with its money to achieve Surface research?
   a) Research grants to individual groups.
   b) Consultants for their labs.
   These are both standard and will produce results.

   Let me suggest something new:
   c) Research grant to two groups who would collaborate on NASA-related Surface problems. (E.g., Barnhill's group and Schumaker's group.)

Why could this be good? Answer: the cross-fertilization would produce more than the sum of the parts. This would be true of both the research and application aspects.

We can explore these thoughts at greater length after I hear from you. Communication· My office phone number is (801), 581-7916 and, if I'm not there, Ms. Sylvia Morris' number is (801), 581-7710. A choice of times to call back would be useful.

Best regards,

Robert E. Barnhill
Professor of Mathematics and
Professor of Computer Science

/smm

cc and thanks: Professor Larry F. Guseman, Jr.

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