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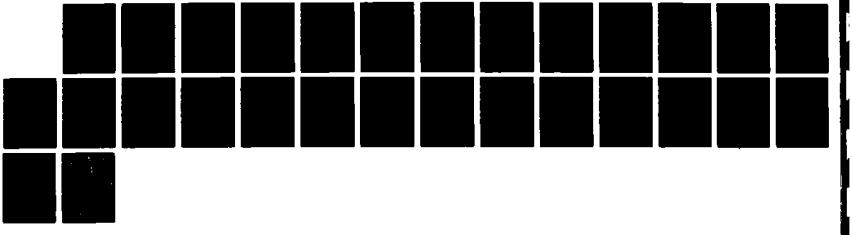

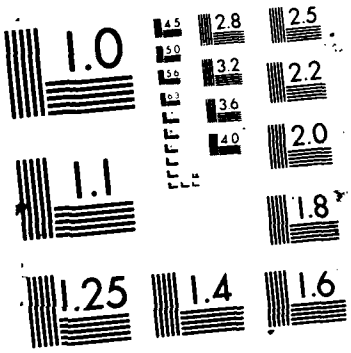
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KNOT SELECTION FOR LEAST SQUARES THIN PLATE SPLINES

by

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Richard Franke

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KNOT SELECTION FOR LEAST SQUARES THIN PLATE SPLINES[#]

John R. McMahon[*]
Richard Franke[+]

Abstract: An algorithm for selection of knot point locations for approximation of functions from large sets of scattered data by least squares Thin Plate Splines is given. The algorithm is based on the idea that each data point is equally important in defining the surface, which allows the knot selection process to be decoupled from the least squares. Properties of the algorithm are investigated, and examples demonstating it are given. Results of some least squares approximations are given and compared with other approximation methods.

Key Words: Knot selection, least squares, thin plate splines, Dirichlet tesselation; scattered data

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1.0 INTRODUCTION

The problem of fitting a surface to small sets of given data has been addressed in many different ways and several computer programs are currently available which enable one to deal with the problem effectively. Many of the methods available involve a global interpolation or approximation scheme and often involves solving a system of equations with an equivalent number of unknowns. For very large sets of data, the problem is computationally intractable. This consideration provides the motivation behind the development of a way to pare the problem down to a more manageable size.

We wish to construct a function F which approximately fits the data since we assume the data collection is subject to measurement error. We propose to use approximation by least squares Thin Plate Splines (TPS), where the surface function is constructed so as to minimize an error function subject to certain constraints. Solving the approximation problem will also involve as many equations as there are data points, but the number of unknowns will be significantly fewer. Part of the appeal of TPS approximation lies in the fact that it minimizes a certain linear functional, and involves a linear combination of functions with no greater complexity than the natural logarithm of the distance function.

Interpolation of scattered data by the method of TPS was developed from engineering considerations by Harder and Desmarais [5]. It can be thought of as a two dimensional generalization of the cubic spline, which models a thin beam under point loads subject to equilibrium constraints. The TPS function is derived

from a differential equation which gives the deformation of an infinite, thin plate under the influence of point loads. A point load is applied at each data point so that the interpolating surface can be constructed as a sum of fundamental solutions of the TPS equation.

In using the least squares TPS approximation method to fit the surface, a fewer number of basis functions than the number of given data points is employed. These basis functions are centered at a different, smaller set of points, which in analogy with the univariate case, we call the knots. Therefore, the problem at hand is one of selecting the knot points, and hence the basis functions. This approach differs from the use of smoothing splines, which were introduced by Wahba and Wendelberger [9] in the multidimensional case, and called Laplacian Smoothing Splines (LSS). LSS minimize a certain functional which is a linear combination of a term measuring fidelity to the data and one measuring smoothness of the function (a generalization of the usual thin plate spline functional). In this case there is still one basis function for each data point, but the interpolation condition is relaxed.

Given a 'large' set of data points, (x_i,y_i,f_i), $i = 1,\ldots,N$, we wish to find a smaller set of knot points, (ξ_j,η_j), $j = 1,\ldots,K$, which will 'represent' the former reasonably well. This could be accomplished by choosing a subset of the original set, or by some process which produces a representative set. The ultimate goal is to approximate the surface from which the original data arose using the representative set. Hence, a surface fit to the large set and one fit to the representative set should

be essentially the same.

Approximation by least squares TPS is straightforward, once the knot points are known. We construct the TPS function

$$F(x,y) = \sum_{j=1}^{K} A_j d_j^2 \log(d_j) + ax + by + c$$

where $d_j^2 = (x-\xi_j)^2 + (y-\eta_j)^2$, and the coefficients A_j are chosen to minimize the error function

$$E = \sum_{i=1}^{N} \{[F(x_i,y_i) - f_i]/s_i\}^2 .$$

The ordinates, f_i, may be subject to random errors, say with standard deviation, s_i, at the i^{th} data point. We model the plate under the point loads at the knot points (as opposed to the data points); therefore the constraint equations for the least squares TPS method, which may be thought of as 'equilibrium conditions' on the plate should be satisfied. Thus, the error function is minimized subject to the constraint equations:

$$\sum_{j=1}^{K} A_j = 0$$

$$\sum_{j=1}^{K} A_j \xi_j = 0$$

$$\sum_{j=1}^{K} A_j \eta_j = 0 \quad .$$

We use LINPACK [1] subroutines to do the actual calculations.

Previous attempts have been made to minimize the error function by considering it to be a function of the knot point locations as well as the coefficients, wherein a total of 3K parameters are involved. As reported on by Schmidt [8], the initial knot configuration was taken to be of tensor product

form. The overall minimization process is a large non-linear one, and is complicated by possible coalescense of knots as well as non-unique solutions (as indicated by consideration of one-dimensional cases). Also, the objective function may have many local minima so that avoiding poor local minima or searching for better local minima may be necessary. Because of these kinds of problems, our goal is to decouple the knot selection process from the least squares process.

When data are somewhat uniformly distributed, methods involving tensor product cubic splines may be desirable. Tensor product methods place knot locations on a grid, which may not reflect the actual disposition of the data points; in fact, there could be no data nearby. Furthermore, even though these problems are surmountable, they could lead to nonuniqueness of solutions and a minimum norm solution that may not be aesthetically appealing.

A different point of view is considered here wherein the knot point locations are predetermined based on two criteria. Specifically, we shall make assumptions relating the density of data to the dependent variable and mandating the importance of each individual data point. Solution of the overdetermined system of equations follows the knot point selection. A summary of the approach and results will be presented. Examples are given which illustrate rather well the ability of the scheme to select knot locations which reflect the underlying density of the data. Actual surface fitting and comparison with two other methods, the Laplacian Smoothing Splines of Wahba and Wendelberger [9], and the tensor product bicubic Hermite method due to Foley [3] are

also reported on.

We also point out two related ideas which are attempts to decrease the number of basis functions to be considered. Each is an attempt to choose a subset of points to be used to construct the approximation. Schiro and Williams [7] used an adaptive process for subset selection and overlapping regions to construct underwater topographic maps. Bozzini, diTisi, and Lenarduzzi [2] gave an algorithm for selecting a subset of points which were important to proper definition of the surface. Both of these methods made no assumptions about the density of the data points relative to the behavior of the surface, and required consideration of the ordinate values.

2.0 THE KNOT SELECTION PROCESS

Given 'a priori' flexibility in knot placement, the problem becomes the selection of knot locations, followed by solution of the system by least squares. Since the selection of knot locations is to be decoupled from the solution of the least squares problem, some assumptions must be made in order to develop an algorithm for the knot selection process. First, we assume that the independent variable data reflects something about the behavior of the dependent variable. For example, the density of the data points may be dependent on the curvature of the surface. Hence, where relatively many data points are found, the function is assumed to be changing behavior rapidly, whereas a low density of data indicates slowly changing behavior. Although this assumption is not universally satisfied in practice, it does not seem to be an unreasonable one.

The second assumption is that each data point is equally important in defining the underlying surface. Therefore the number of data points represented by each knot should be the same or nearly the same. This leads to 'equal representation' of the data points by the knot points where each data point is 'close' to a knot point. A key advantage achieved in pursuing this approach is the existence of a natural heuristic for moving the knots around the plane in searching for a good knot configuration. This point will be elaborated on later in the paper.

Our knot selection algorithm is based on these last two assumptions. First, we wish to minimize the sum of the distances squared from each data point to the nearest knot point; that is, minimize the 'global' value,

$$GN^2 = \sum_{i=1}^{N} \min_{j} \left[(x_i - \hat{x}_j)^2 + (y_i - \hat{y}_j)^2 \right]$$

This function is continuous and piecewise quadratic. The expression leads naturally to a 'default' Dirichlet Tesselation, a partitioning of the plane with respect to the knot points (see Figure 1). Thus, we say each data point belongs to some knot point according to the Dirichlet tile in which it lies. Data points on any of the tile boundaries (ties) must be resolved by a determination of which tile they belong to or some sharing mechanism. Our initial guess at the knot point configuration was taken to be quasi-gridded.

Differentiation of GN^2 with respect to the $\hat{x}_j$ and $\hat{y}_j$ show that at the minimum, each knot point will occupy the centroid with respect to the data points inside that tile. Given the

initial configuration of knot points with its Dirichlet Tesselation, the following algorithm for iteration to a local minimum GN^2 value is employed:

(a) compute the centroid of each tile with respect to the data points contained within each tile;

(b) move the knots to the corresponding centroids, which results in a new Dirichlet Tesselation and a new set of knot point - data point associations; this is the configuration for the next iteration.

(c) quit when two successive iterations yield the same knot locations, which means that a local minimum value of GN^2 has been found.

This algorithm was formulated in discussions at the Istituto per le Applicazioni della Matematica e dell'Informatica in 1983 [10], after the problem was posed by G. Nielson and R. Franke.

We note that the value of GN^2 will necessarily decrease as the iterations continue, until two successive iterations yield the same configuration; this will be proven below. In the case where no data points lie in a tile for some knot point, the knot point is moved to the nearest data point. This mechanism avoids knots without data points. Futhermore, if a data point lies on a tile boundary, it is assigned to the knot with the smallest subscript (amongst the appropriate choices of knot points). Employment of a different criterion for the resolution of ties may yield different results. We note that knots cannot coalesce.

The following theorem is pertinent to this algorithm.

Theorem: The function GN^2 decreases with each iteration which involves movement of a knot point.

Proof: Write GN^2 in the more convenient form

$$GN^2 = \sum_{j=1}^{K} \sum_{i \in I_j} [(x_i - \xi_j)^2 + (y_i - \eta_j)^2] \qquad (1)$$

where $I_j = \{i: (x_i,y_i)$ in the tile for $(\hat{x}_j,\hat{y}_j)\}$. In (1), the interior sum is the sum of the distances squared from the data points in a tile to the knot point in that tile, and the exterior sum is over all K of the tiles. Let a prime denote the new knot points and index sets. This form leads to the expressions

$$(x'_j,y'_j) = \left(\sum_{i \in I_j} x_i/n_j, \sum_{i \in I_j} y_i/n_j \right),$$

where n_j is the number of indices in the set I_j. The new knot points will lead to a new tesselation, followed by the new index sets I'_j. Then the expression (1) is greater than or equal to

$$\sum_{j=1}^{K} \sum_{i \in I_j} [(x_i-\hat{x}'_j)^2 + (y_i-\hat{y}'_j)^2] \qquad (2)$$

because the new knot point locations minimize the contribution of the interior sums. This expression (2), in turn, is greater than or equal to

$$\sum_{j=1}^{K} \sum_{i \in I'_j} [(x_i-\hat{x}'_j)^2 + (y_i-\hat{y}'_j)^2] \qquad (3)$$

since an index i moves to another set only in the case wherein the corresponding data point is now closer to a different knot point, thus decreasing its contribution to the global GN^2 value.

Finding a local minimum of GN^2 is well-served by this algorithm; however, as seen in a one dimensional example [6], the function GN^2 is rife with local minima, and the local minimum value found depends on the initial configuration of knots used. We can draw similar conclusions for the multidimensional case based on the one dimensional analogy.

The process of locating each knot occurs in two distinct steps: first, each data point is assigned to the closest knot

and second, a determination is made within each tile as to the location of its centroid. As a direct result of the centroid requirement, the GN^2 function will stabilize at the local minimum value corresponding to the particular quadratic piece on which the knot is found.

The local minimum value will frequently occur out of the domain of the corresponding quadratic piece. This leads to a 'cascading' phenomenon which continues until a local minimum value is attained. However, the global minimum value will not necessarily be attained since the cascading will stop as soon as a local minimum value is found within the domain of each quadratic piece.

This inconsistent performance of the algorithm in finding the global minimum value of GN^2 leads to consideration of a somewhat different criterion for locating a good configuration of knot points. We wish to exploit the second assumption specified earlier, while taking advantage of the minimization of the GN^2 function. Since each data point is assumed to be equally important, the Dirichlet tile for each knot should contain about the same number of data points. Thus, we wish to minimize the sum of the squares of the differences between the number of knots in each tile and the average number of data points that should belong to each tile; that is, minimize the quantity

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

The new algorithm for determining knot locations is based on the minimization of D, subject to the constraint that each knot be located at the centroid of its tile.

This new optimization leads to a natural heuristic for moving knots from a stable configuration to a possibly better configuration. We call the current configuration of knots a 'base' configuration, and iterate through the algorithm as follows:

(a) generate a new guess for the knot locations by moving the knot(s) with the smallest number of data points in their tile(s) toward the knot(s) with the largest number of knot(s) in their tile(s); the distance moved is initally a large fraction of the total distance between the knots.

(b) iterate to a stable configuration using the first algorithm, compute the values of GN^2 and D, and compare D to the smallest value achieved to date, as represented by that of the base configuration;

(c) repeat the process above when a smaller value of D is obtained, with the present configuration as the base configuration;

(d) when a smaller value of D is not found, take a shorter step in the movement of the knot(s) and repeat the process above;

(e) continue with smaller and smaller steps until a smaller value of D is found (or an equal value of D with a smaller GN^2 value) or until the knot locations return to the base configuration;

(f) perform the search in the symmetrical way when the base configuration is returned to; that is, move the knot(s) with the largest number of data points in their tiles toward the knot(s) with the smallest number of points in their tile;

(g) quit when no smaller value of D is found.

The movement of the knots is justified by the rationale that a more equitable distribution of data points can be found by moving the tile boundaries across data points. Note that the algorithm for computing a local minimum of the GN^2 function value is embedded in this new algorithm.

3.0 RESULTS AND EXAMPLES

Using our algorithm for the a priori selection of the knot

point locations, experiments were conducted to test the scheme using different sets of test data. This was followed by verification of the scheme on a large set of real data. Results from two sets of the test data are presented here: one consisting of 200 data points called 'Cliff', and one consisting of 500 data points called 'Humps and Dips'. Both sets of data were generated using known functions (see Franke [4]) in a way that forced the density of points to be proportional to the curvature of the sampled function. Figures 2-5 show these two test data sets graphically, and illustrate the optimized knot point configurations found using the least squares algorithm. Figure 6 depicts actual hydrographic data collected in Monterey Bay, with greatly varying density. Figure 7 shows the results of applying the algorithm with 100 knots, and is particularly interesting because the density of the data is faithfully replicated by the knots. We note that the assumption regarding the density of the data points being indicative of the behavior of the dependent variable is not actually satisfied in this case, due to the source of the data. Nonetheless, these results demonstrate the ability of the algorithm to produce representative sets of knots.

We also investigated how closely the constructed surface F and the 'true' surface resemble one another. This comparison is made in the context of the root-mean-squared error (RMS) of the residuals (at the data points) and on a rectangular grid of locations in the plane. The two data sets constructed above, and one other which was generated in a similar manner, were used to compare RMS errors for the least squares algorithm developed here

with the method of Wahba and Wendelberger (Laplacian Smoothing Splines), and the method of Foley (Bicubic Hermite Tensor Product Splines).

The dependent variable values of the experimental data sets were generated in two ways: 1) using a known function, and 2) contaminating the known function by the injection of independent, identically distributed normal random errors with a specified composite standard deviation of 0.05. The actual standard deviation was about 0.0485. In the first case, we would expect the RMS error on the data points and on the grid to be about the same, and to decrease as the number of knot points used to represent the data is increased.

In the contaminated case, the dependent variable at each data point is the sum of the unknown underlying function value and the error function value so that the difference between the constructed surface and the 'true' surface is mainly attributable to the presence of error in the data. In the best situation, we expect the RMS error in the residuals to match the composite standard deviation of the random error injected to obtain the contaminated data. At the grid points, we expect the RMS error to be smaller than the composite standard deviation, since the grid sample is larger (33*33) and the errors are distributed more evenly throughout the entire region of interest.

Some observations can be made regarding Tables 1-3. The general trend of the RMS error on both the data points and the grid is to diminish as the number of knot points is increased. As expected with the exact data, the RMS error of the residuals and the RMS error on the grid are roughly equivalent. For the

contaminated data, the RMS error of the residuals roughly matches the composite standard deviation of the data, and the RMS error on the grid is smaller than the RMS error of the residuals, as expected. In Table 1, the errors over the grid increase as the number of knot points is increased, and the RMS value of the residuals becomes less than the composite standard deviation of the injected errors. In this case, undersmoothing has occurred, and the surface is "drawing" toward the error.

In comparing least squares TPS to the smoothing spline method in the exact data case, we note that the smoothing spline method yields a residual RMS error of 0. This could be expected, since there is no error in the data and the spline of interpolation is chosen. On the grid, the RMS error is small. When the data is not contaminated, the RMS error of the least squares algorithm only begins to become as small as that of the smoothing splines method when the number of knots used becomes large. We also note that in the 500 data point set, no comparison is made since a potential limit for computing smoothing splines is 200-300 data points.

Foley's method for the contaminated case gives errors nearly equal to the composite standard deviation of the errors injected into the data. However, on the grid, the least squares method does better, an indication that smoothing is occurring, as expected. We also note that an increase in the number of grid points does not significantly improve the RMS error in Foley's method, even though an increase in the number of knots in the least squares method usually yields improved results. We used the default local approximations in Foley's method, and we note

that performance of the method may be improved by using lower degree local approximations to estimate the grid values to be used.

Finally, we note that the search for a best knot configuration can turn out to be rather expensive. For a large number of data points with a moderately large number of knot points, the computational effort could be excessive, although we are investigating ways of speeding up the algorithm. Furthermore, as we noted earlier, the end results are dependent on the initial guess, although they generally look quite good for any reasonable initial guess.

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METHOD	NUMBER OF DATA POINTS/ KNOT POINTS	NO ERRORS IN DATA		CONTAMINATED DATA	
		RESIDUAL	GRID	RESIDUAL	GRID
LSTPS	200/20	0.01562	0.01474	0.05214	0.01795
LSTPS	200/25	0.01179	0.01154	0.04805	0.02040
FOLEY	200/5x5	0.00777	0.00613	0.05996	0.04819
LSTPS	200/35	0.00626	0.00616	0.04590	0.02146
FOLEY	200/6x6	0.00512	0.00417	0.05113	0.03745
SMOOTHING	200	0.0	0.00096	0.04272	0.01806

Table 1: Comparison of RMS errors on 'CLIFF' 200 points

METHOD	NUMBER OF DATA POINTS/ KNOT POINTS	NO ERRORS IN DATA		CONTAMINATED DATA	
		RESIDUAL	GRID	RESIDUAL	GRID
LSTPS	200/20	0.05525	0.05465	0.07571	0.05866
LSTPS	200/25	0.02520	0.02646	0.05603	0.03385
FOLEY	200/5x5	0.01206	0.01332	0.04819	0.04965
LSTPS	200/35	0.01662	0.01843	0.05274	0.02853
FOLEY	200/6x6	0.00968	0.01144	0.05028	0.03962
SMOOTHING	200	0.0	0.00254	0.03900	0.02789

Table 2: Comparison of RMS errors on 'HUMP AND DIPS' 200 points

METHOD	NUMBER OF DATA POINTS/ KNOT POINTS	NO ERRORS IN DATA		CONTAMINATED DATA	
		RESIDUAL	GRID	RESIDUAL	GRID
LSTPS	500/20	0.02402	0.02517	0.05256	0.02738
LSTPS	500/25	0.01664	0.01766	0.04818	0.02283
FOLEY	500/5x5	0.01346	0.01230	0.05844	0.03767
LSTPS	500/50	0.00645	0.00845	0.04544	0.01961
FOLEY	500/7x7	0.00645	0.00552	0.05696	0.04864

Table 3: Comparison of RMS errors on 'HUMPS & DIPS' 500 points

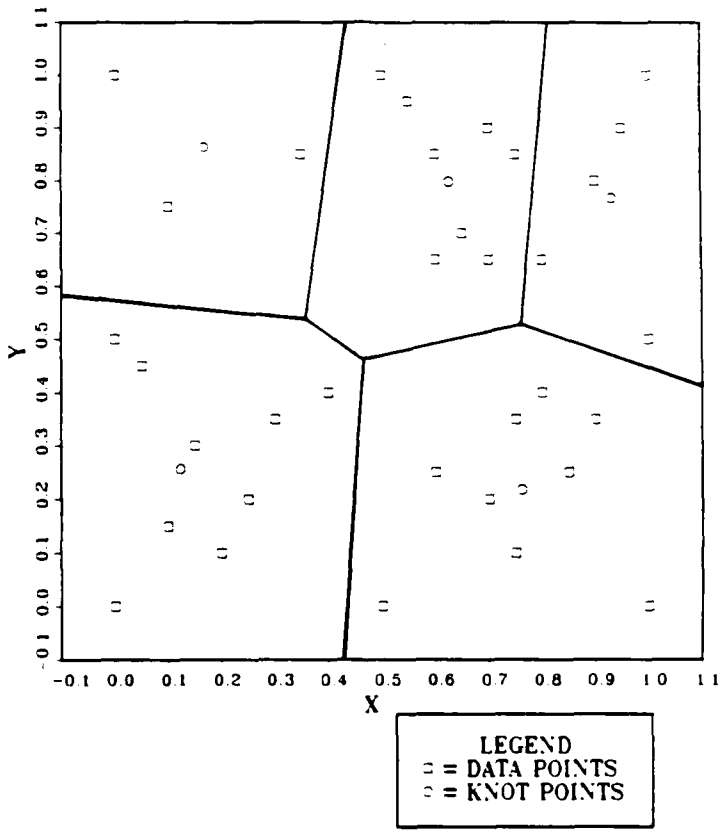

Figure 1: A Dirichlet Tesselation with 5 Tiles. It is constructed by connecting the perpendicular bisectors of the lines joining each of the knot points.

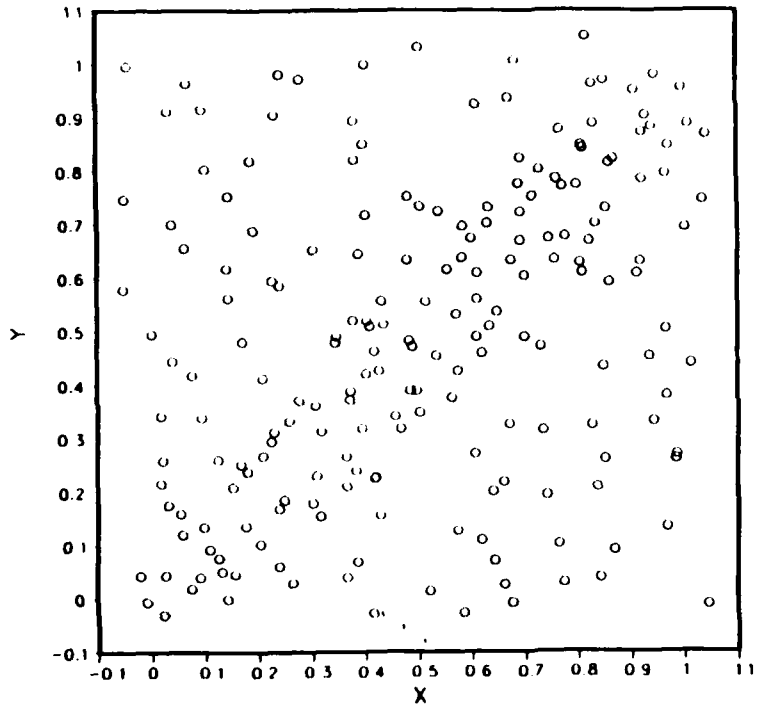

Figure 2

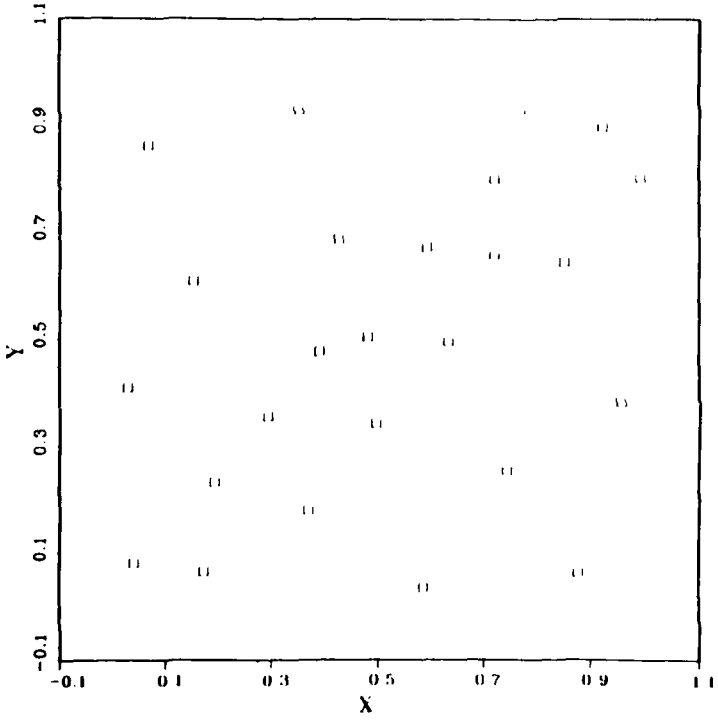

Figure 3

Figures 2 and 3: The 'Cliff' data set. Note the relatively dense disposition of data points across the diagonal where the underlying surface drops off. The 25 knot points used clearly reflect the behavior of the data set, as expected.

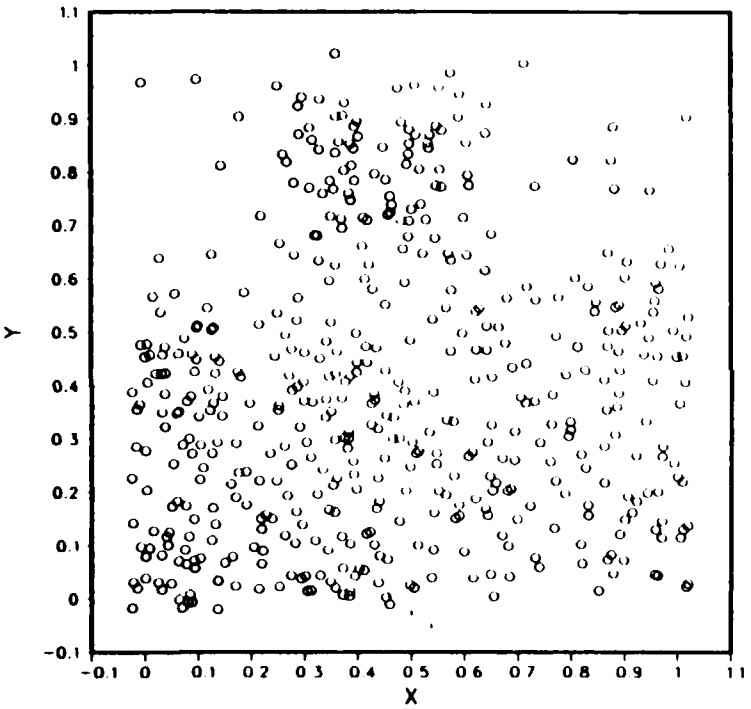

Figure 4

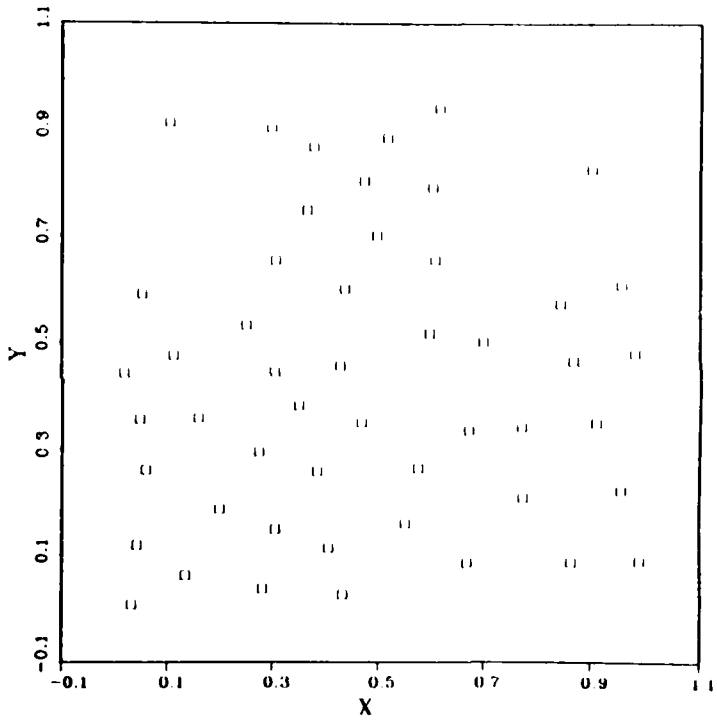

Figure 5

Figures 4 and 5: The 'Humps and Dips' data set. Note how clumps of data appear in three portions of the plane, indicating that the underlying surface is undergoing change. A set of 50 knot points was used to represent the data.

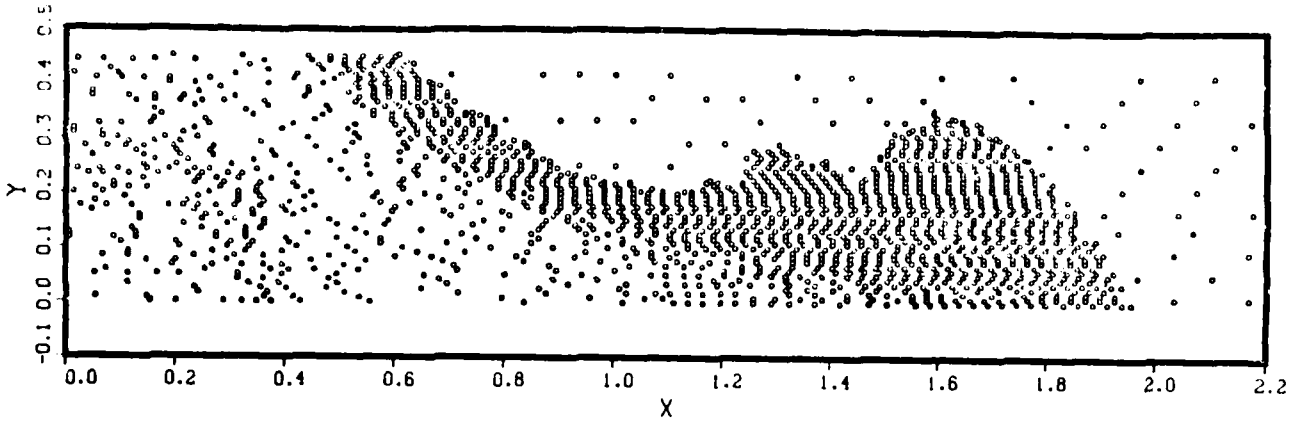

Figure 6

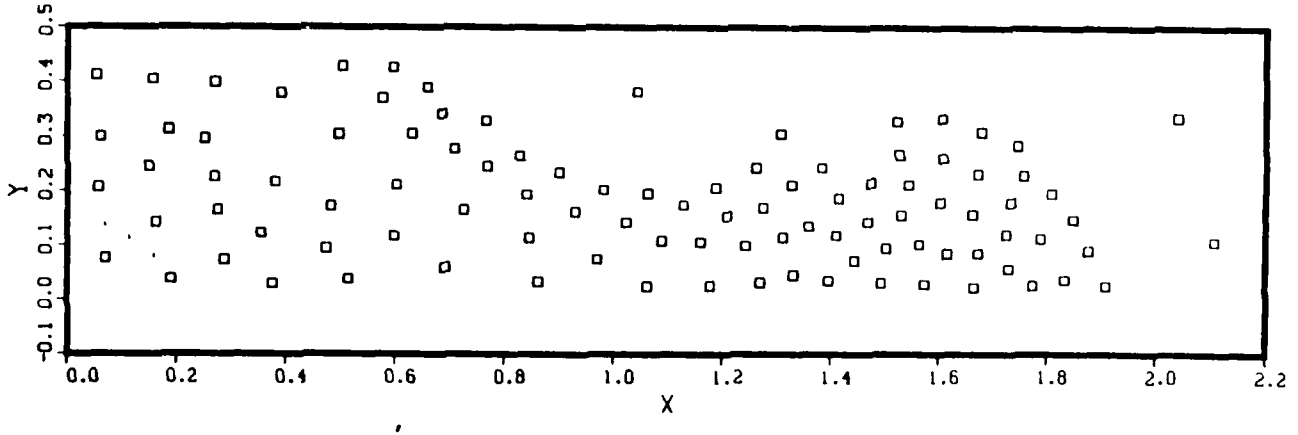

Figure 7

Figures 6 and 7: Hydrographic Data from Monterey Bay, Ca. Here, 1669 data points (soundings) are represented by 100 knot points. The results are very reasonable.

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