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A study of methods for estimating parameters in rational polynomial models

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A STUDY OF METHODS FOR ESTIMATING PARAMETERS

IN RATIONAL POLYNOMIAL MODELS

BY

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ABSTRACT

The use of rational polynomials for approximating surfaces is investigated in this study. In particular, methods for estimating parameters for a rational polynomial model were investigated.

A method is presented for finding initial estimates of the parameters. Two iterative methods are discussed for improving those estimates in an attempt to minimize the sum of the squares of the residuals. These two methods are (1) Scarborough's Method for applying the theory of least squares to nonlinear models and (2) the Method of Steepest Descent.

Data from two functions were chosen and approximated as illustrations. Each set of data was used two ways, (1) as generated, and (2) with random errors added, thus giving four examples.

Scarborough's Method for improving the starting values was very effective, for the examples chosen, and the approximations were excellent. The study indicates, therefore, that rational polynomials have good potential as useful functions for surface approximants.

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CHAPTER I

INTRODUCTION

Almost as long as man has had experimentally determined data he has needed to construct approximating functions that would correlate these data, with an acceptable degree of accuracy, so that analysis of an associated problem could proceed. The need is even more dire today for at least two good reasons. (1) There is, in some areas, a great deal of data available needing critical analysis. (2) In other areas, data are difficult to obtain and hence scarce, nevertheless requiring satisfactory methods of analysis.

Without some means of correlating past results with present needs or present results with future needs each new response must be found by sampling and evaluating. The more information that can be obtained from presently accumulated data and the more costly the process of sampling and evaluating at every new observation point becomes, the more important approximating functions become.

When data are collected experimentally no exact function, F, is known nor can be known which perfectly correlates such data. A model of F may be known experimentally but its parameters may remain unknown. Or, even if a very accurate approximant for F is known, it may be so complicated or difficult to evaluate that it is not expedient to use. In any of these cases, therefore, an approximating function, G, is important.

For most applications, if Z is a function of two independent variables, x and y, for some range of the independent variables, the locus of Z is, in general, a surface. Therefore, the problem of approximating Z is generally a problem of surface fitting and this study shall consider only this situation.

Assume, therefore, that a function, G(x,y), is desired to approximate Z for some region, R, of the xy plane for which Z = F(x,y), i.e.,

$$G(x,y) \approx Z = F(x,y). \tag{1.1}$$

The author shall herein investigate the use of rational polynomials as a surface approximating device.

G(x,y) is a rational polynomial if

$$G(x,y) = N(x,y)/ D(x,y) \tag{1.2}$$

where N(x,y) and D(x,y) are polynomials. Specifically

$$N(x,y) = \sum_{i=0}^{K} \sum_{j=0}^{K-i} A_{ij} x^i y^j \tag{1.3}$$

and

$$D(x,y) = \sum_{i=0}^{L} \sum_{j=0}^{L-i} B_{ij} x^i y^j . \tag{1.4}$$

This study shall concentrate on an appropriate method of estimating the parameters, A_{ij} and B_{ij}, using discrete samples Z_n, from the region R. An attempt shall be made to find a suitable procedure to minimize

$\sum_{n=1}^{N} \left[Z_n - G(x_n,y_n)\right]^2$ for any number, N, of discrete sample points.

The study shall be made for two types of data and for two classes of functions, $F(x,y)$. First, a study shall be made using data taken from tables or generated from known functions such that no significant errors are included, i.e., Z_n is known to correctly represent $F(x_n,y_n)$ within a certain number of places of accuracy. Approximations shall be examined using these "errorless" samples when $F(x,y)$ is a member of the family of $G(x,y)$ and when it is not a member thereof.

The second type of Z_n used shall contain errors, i.e., $Z_n = F(x_n,y_n) + e_n$. This type Z_n shall represent data that are collected during some experimental process where measurements are subject to errors. The errors considered herein shall be restricted to relatively small, random errors with an expected value of zero. The approximations of both classes of functions, those for which $F(x,y)$ is a member of the family of $G(x,y)$ and those for which it is not, shall be examined using this type data, also.

In summary, a method for estimating parameters of rational polynomials so that the sum of the squares of the residuals will be a minimum shall be attempted using sets of data "with" and "without" errors for both a class of functions which are members of the family of the approximant and for a class of functions which are not members thereof.

Before considering the choice of rational polynomials as a device for approximating surfaces, consider for a moment the related problem of curve fitting. Curve fitting, in the past, has mostly been limited to the use of polynomials, or at best, polynomials and a few transcendental functions.

Several excellent techniques have been developed for estimating the parameters of these functions including methods for using the theory of least squares to determine the "best fit" with the model selected. Surface fitting has largely been an extension of these ideas and techniques using the same type functions.

With the introduction and more common use of large high speed computers other functions for curve fitting are being examined. One of these is rational polynomials. These functions have been hailed by such noted analysts as Hamming[(1)], Thacher and Tukey[(2)], and others as having many advantages. The study of rational polynomials as useful functions for surface approximations seemed, therefore, a logical choice in attempting to extend the ideas of surface fitting beyond their present bounds.

CHAPTER II
GENERAL REVIEW OF LITERATURE

There are apparently no publications available which deal directly with the use of rational polynomials for surface fitting. There are certain related materials, however, which make a contribution in this area.

Hamming[1] devotes an entire chapter to rational functions. He discusses their use for curve fitting through points equal in number to the number of parameters of the model and lists several of their advantages. He implies that the functions have good possibilities for development into useful approximants.

Thacher and Tukey[2] discuss the merits of rational polynomials for curve fitting and interpolation. They appear very enthusiastic about the flexibility of rational polynomials and attribute to them qualities superior, in many ways, to regular polynomials. Their results indicate that their conclusions are justified.

Almost any textbook on numerical analysis has some discussion of the theory of least squares and its use. Hildebrand[3] devotes an entire chapter to the subject. His discussion of "Least-squares Approximation over Discrete Value Ranges" is very good. His explanation of obtaining the normal equations is unusually clear.

Scarborough's[4] discussion of the theory of least squares adds a general method for the theory's use with nonlinear models. His method is discussed in detail later in this study. His "Method of Averages" for making initial estimates of the parameters in nonlinear models is used, also.

Kunz[5], in his text on numerical analysis, suggests using the Method of Steepest Descent for solving nonlinear sets of equations. He includes a discussion of the method and its use.

The criteria for judging "best fit" with a particular model depend upon the author consulted. Hamming,[1] for instance, lists four choices. The theory of least squares was chosen for this study because it is probably the most widely used. This is especially true when randon errors are apt to be contained in the data.

CHAPTER III

DISCUSSION

A. THE GENERAL PROBLEM.

The first step in using a rational polynomial for approximating a surface is selecting a model. This is often a major problem and appears worthy of its own investigation. It is not the purpose of the author to solve this problem at this time.

The general form of the approximant is

$$G(x,y) = \frac{A_{00}+A_{10}x+A_{01}y+A_{20}x^2+A_{11}xy+\ .\ .\ .\ +A_{OK}y^k}{B_{00}+B_{10}x+B_{01}y+\ .\ .\ .+B_{OL}Y^L}. \quad (2.1)$$

In order that the estimation of parameters may be unique one parameter must be eliminated. It is convenient to define $B_{00} = 1$. Thus equation 2.1 becomes

$$G(x,y) = \frac{A_{00}+A_{10}x+A_{01}y+\ .\ .\ .+A_{OK}y^K}{1+B_{10}x+B_{01}y+\ .\ .\ .+B_{OL}y^L}. \quad (2.2)$$

Substituting Z for G(x,y), equation 2.2 can be rearranged as follows:

$$A_{00}+A_{10}x+A_{01}y+ \ldots +A_{OK}y^K - Z(B_{10}x+B_{01}y+ \ldots +B_{OL}y^L)\approx Z. \quad (2.3)$$

If x, y and Z are known for a set of discrete points equal to or greater in number than the number of parameters, the equations formed by inserting these data in equation 2.3 become a system in which the parameters are the unknowns. If this system is solved using data points equal in number to the number of parameters the resulting function, $G(x,y)$, using the parameters thus found will pass through each of the data points used. This is of no particular value for approximating a surface containing other points throughout the region, R, except for the special case to be discussed next.

In the special case where the true model, $F(x,y)$, is a member of the family of the approximating model, $G(x,y)$, and the observations, Z_n, are "errorless," the parameters found (using data points equal to the number of parameters) will be those which form the function, $F(x,y)$, and the fit will be "exact" throughout the region, R.

If $F(x,y)$ is not a member of the family of $G(x,y)$, or if there are errors in the data, data points equal in number to the number of parameters are not adequate for a general fitting of the surface throughout the region, R.

It would seem rare indeed to have enough knowledge about the function, $F(x,y)$, and about the data, Z_n, to recognize the special case in advance. If the special conditions do apply, a general solution will give the proper parameters also, with only slightly more work. Therefore, the procedure for a more general solution will usually be followed from the beginning.

As was stated before, the theory of least squares shall be used as the criterion for judging the "best fit" of the surface with a given model, $G(x,y)$. According to this theory "best fit" has been attained when the sum of the squares of the residuals is a minimum.

There appears to be no simple or direct method for applying the theory of least squares to a function that is nonlinear in its parameters. Two methods which can be used were investigated. Both were iterative processes requiring an initial estimate of the parameters for starting values with subsequent efforts being made to improve those estimates. Each improvement was based upon the last value obtained, thus forming the iterative process.

One of these methods is outlined by Scarborough[(4)] and shall subsequently be referred to, in this paper, as "Scarborough's Method" for improving initial parameters. The other method investigated was the "Method of Steepest Descent" and shall be referred to by name. Both methods are very dependent upon the initial estimates of the parameters. For some choices the iterative processes converge very quickly, for others, they converge very slowly or not at all. Therefore, an effective method of obtaining starter values is very important.

B. METHODS FOR OBTAINING INITIAL ESTIMATES

The method which most consistently gave initial estimates of parameters which ultimately led to convergence is presented next.

First, a set of equations is found, using equation 2.3, employing points, (x_n, y_n, Z_n), greater in number than the number of parameters to be determined. The set would appear as follows:

$$A_{00}+A_{10}x_1+A_{01}y_1+ \cdots +A_{0K}y_1^K - Z_1(B_{10}x_1+B_{01}y_1+\cdots +B_{0L}y_1^L)=Z_1$$
$$A_{00}+A_{10}x_2+A_{01}y_2+ \cdots +A_{0K}y_2^K - Z_2(B_{10}x_2+B_{01}y_2+\cdots +B_{0L}y_2^L)=Z_2$$
$$\vdots$$
$$A_{00}+A_{10}x_n+A_{01}y_n+\cdots+A_{0K}y_n^K - Z_n(B_{10}x_n+B_{01}y_n+\cdots+B_{0L}y_n^L) = Z_n. \tag{2.4}$$

To these equations apply the theory of least squares for finding parameters, i.e., form the general set of normal equations and solve them simultaneously. The values thus found are, in general, more dependable than those given by any other method investigated.

If successive iterations do not lead to convergence using these starting values a new set may be obtained by increasing or decreasing the number of data points used or by selecting other data points from the region, R.

It may appear to the casual observer that the initial estimates found for the parameters, using the method presented, will minimize the sum of the squares of the residuals since the "least squares" technique was used to obtain these values. This is not generally true.

The reason the method presented does not minimize the sum of squares of the residuals for the general case can be seen by inspecting that sum and the sum being minimized by the method presented.

The sum of the squares of the residuals is given by

$$\sum_{n=1}^{N}\left[\frac{Z_n - N(x_n,y_n) + Z_n\cdot d(x_n,y_n)}{1 + d(x_n,y_n)}\right]^2 \tag{2.5}$$

where $d(x,y) = D(x,y) - 1$.

The sum being minimized by the method presented for finding initial estimates of the parameters is given by

$$\sum_{n=1}^{N} \left[Z_n - N(x_n,y_n)+Z_n \cdot d(x_n,y_n) \right]^2 \qquad (2.6)$$

It is evident, from these equations, that the parameters which minimize equation 2.6 will not, in general, be the parameters which minimize equation 2.5, except for the special case previously discussed.

An additional method, referred to as "The Method of Averages," is given by Scarborough[4]. This simply requires that equations 2.4 be divided into groups equal in number to the number of parameters to be found. (The number in each group need not be equal.) The equations in each group are summed, thus forming a set of equations, which can be solved simultaneously for the parameters.

C. IMPROVING THE ESTIMATES.

"Scarborough's Method" for applying the theory of least squares to a general case of a nonlinear model can be adapted to rational polynomials as follows:

Consider Z_n a function of the parameters, i.e.,

$$Z_n = G(x_n,y_n,A_{ij},B_{ij}) + e_n \qquad (2.7)$$

with A_{ij} and B_{ij} defined as the ideal parameters for minimizing the sum of squares of the residuals and e_n defined as the error in any approximation. Assume the initial estimates of the parameters have been found and are identified as $A_{ij}^{(1)}$ and

$B_{ij}^{(1)}$. Define the corrections needed to make each starting value equal to the corresponding ideal value as α_{ij} and β_{ij}. Thus

$$A_{ij} = A_{ij}^{(1)} + \alpha_{ij} \tag{2.8}$$

and

$$B_{ij} = B_{ij}^{(1)} + \beta_{ij}. \tag{2.9}$$

By substitution,

$$Z_n = G(x_n, y_n, A_{ij}^{(1)} + \alpha_{ij}, B_{ij}^{(1)} + \beta_{ij}) + e_n. \tag{2.10}$$

Expanding this function by "Taylor's Theorem of Several Variables" about the starting values it becomes

$$Z_n = G(x_n, y_n, A_{ij}^{(1)}, B_{ij}^{(1)}) + \sum_{i,j} \alpha_{ij} \left(\frac{\partial G}{\partial A_{ij}}\right)_n + \sum_{i,j} \beta_{ij} \left(\frac{\partial G}{\partial B_{ij}}\right)_n + \delta_n. \tag{2.11}$$

The first term $G(x_n, y_n, A_{ij}^{(1)}, B_{ij}^{(1)})$ is the first approximation of Z_n and shall be identified hereafter as $Z_n^{(1)}$. Thus the expansion becomes

$$Z_n = Z_n^{(1)} + \sum_{i,j} \alpha_{ij} \left(\frac{\partial G}{\partial A_{ij}}\right)_n + \sum_{i,j} \beta_{ij} \left(\frac{\partial G}{\partial B_{ij}}\right)_n + \delta_n. \tag{2.12}$$

with δ_n now containing the additional error caused by truncating the series after the first order terms.

These equations are linear in the corrections α_{ij} and β_{ij} and may be dealt with by the method of least squares to find the "best" corrections.

The sum of the initial parameters and the corrections, $A_{ij}^{(1)} + \alpha_{ij}$ and $B_{ij}^{(1)} + \beta_{ij}$, may then be treated as new starting values. This iterative process may be carried on until the corrections are no longer significant. Hopefully, the parameters will then be those for which the sum of squares of the residuals, $\sum_{n=1}^{N} \left[Z_n - G(x_n, y_n)\right]^2$, is a minimum.

A discussion of the "Method of Steepest Descent" can be found in Kunz[5], and several other texts, and shall not be repeated here.

Both methods were used in attempting to solve the example problems which follow and comments shall be included concerning their respective effectiveness.

D. THE CHOICE OF FUNCTIONS FOR THE EXAMPLES AND THE PREPARATION OF DATA.

Two functions were chosen for generating data to be approximated as illustrations. The first function chosen was

$$Z = F(x,y) = \frac{3 + 2x + 4y + 5xy}{1 + x^2 + y^2} \tag{2.13}$$

and the second function chosen was

$$Z = F(x,y) = 1 - e^{-xy}. \tag{2.14}$$

The function chosen for the approximant in both cases was

$$G(x,y) = \frac{A_{00}+A_{10}x+A_{01}y+A_{20}x^2+A_{11}xy+A_{02}y^2}{1 + B_{10}x+B_{01}y+B_{20}x^2+B_{11}xy+B_{02}y^2} \tag{2.15}$$

The first function, equation 2.13, is a member of the family of the approximant, G(x,y), and the second function, equation 2.14, is not. It is obvious, therefore, that a "fit" exists for the first function. The existence of a good "fit" for the second function is not obvious. The second function, therefore, should supply the better test of the effectiveness of rational polynomials as approximants.

Data was generated using both functions, equations 2.11 and 2.12, from the region, R, $0 \leq x \leq 3$, and $0 \leq y \leq 2$. In each case the x and y values were both incremented from zero to their upper bound by intervals of twenty-five hundredths (.25) thus giving 117 discrete data points with their responses. This was done with an IBM 1620 and a card was punched for each point containing x_n, y_n, and Z_n.

To simulate data with random errors in the responses for the same functions and over the same region, R, a program was written to read the data from each card, add an error, taken at random within a predesignated range, to each response and a card punched for each point containing x_n, y_n, ZE_n, and ZT_n. ZE represents the response with random error added and ZT represents the true response as originally generated.

The errors added to the responses were bounded as follows:

(1) The absolute value of any error, e_1, added to a response from the first function must be less than or equal to one-half, i.e., $|e_1| \leq 1/2$. This represents a possible error of 14.4% of the mean value of the true responses.

(2) The absolute value of any error, e_2, added to a response from the second function must be less than or equal to one-tenth, i.e., $|e_2| \leq 1/10$. This

represents a possible error of 17.2% of the mean value of the true responses.

These four sets of data represent all the cases outlined.

To assure random selection from each set of data thus generated, each set was shuffled as one would shuffle playing cards. The data used were from these shuffled sets and were reshuffled from time to time.

E. THE EXAMPLES AND THEIR SOLUTION.

EXAMPLE I. The first attempt to determine parameters was made using "errorless" data generated from equation 2.13. This is, of course, the special case referred to in the general discussion and good results were expected. This provided an opportunity for checking the programs used since the results could be anticipated.

First, a system of equations was formed and solved using eleven data cards. This was the minimum number possible because the approximant, equation 2.15, has eleven parameters. This was repeated several times. These systems of equations, as well as all others, were solved by the Gauss-Jordan Method as outlined by Kunz[5] and others. The program for this method was taken from the M.S.M. Computer Center Library.

The parameters determined for each of these systems were, as expected, the coefficients of the function from whence the data were generated. Accuracy was approximately to four decimal places. Errors were only those accumulated by the computer through round-off and the reduction method used.

The second program tried was one to find starting values by the method presented in this study. Again, each attempt gave the expected parameters. The only noticeable change was the loss of one decimal place accuracy when 99 data cards were used. This was to be expected due to the large number of operations performed in forming the coefficients.

The third program checked was the one for finding starting values by the "Method of Averages." Three equations from equation 2.4 were summed to form each equation of the set of eleven equations needed. This was repeated using groups of five and nine to form the eleven equations. The results in each case gave approximately the same values for the parameters as were obtained by passing the surface through eleven points.

An attempt to improve some of the initial parameters, found by the above methods, was made using the "Method of Steepest Descent." This was futile with the restrictions imposed upon the method. A brief description of those restrictions is given next.

The direction numbers required to determine the path of steepest descent and thus reduce the sum of the squares of the residuals are given by

$$\sum_{n=1}^{N}(Z_n - Z_n^{(1)})\frac{x_n^{\,i} y_n^{\,j}}{D_n^{(1)}} \qquad (2.16)$$

for any parameter A_{ij}, and are given by

$$-\sum_{n=1}^{N}(Z_n - Z_n^{(1)})\frac{x_n^{\,i} y_n^{\,j} Z_n^{(1)}}{D_n^{(1)}} \qquad (2.17)$$

for any parameter B_{ij}. (B_{00} was defined to be 1.) The magnitude of the correction of the parameters is arbitrary but these were the restrictions imposed:

> The direction cosines were found and movements were tried beginning with eight times each direction cosine. If the sum of the squares of the residuals was not reduced with this choice the amount was divided by two and this was tried. This was repeated until the last attempt employed only one-eighth each direction cosine. If this amount would not reduce the sum of the squares of the residuals the program would automatically exit.

"Scarborough's Method" for improving the parameters produced a small surprise. One additional decimal place of accuracy, in addition to the four previously given, was always added and sometimes two. This had not been expected with the accuracy already given, and it indicated that the method had excellent possibilities.

The primary equation necessary for using Scarborough's Method is equation 2.12. The expansion of this equation, 2.12, for the approximant used, 2.15, is

$$A_{00}+A_{10}x_n+A_{01}y_n+A_{20}x_n^2+A_{11}x_ny_n+A_{02}y_n^2$$
$$- Z_n^{(1)}(B_{10}x_n+B_{01}y_n+B_{20}x_n^2+B_{11}x_ny_n+B_{02}y_n^2) \;/\; D_n^{(1)} \approx Z_n-Z_n^{(1)} . \qquad (2.18)$$

The insertion of data values into this equation forms a set of equations equal in number to the number of data cards used. The normal equations used for a "least squares" solution are then formed using this set of equations as defining the residuals. The corrections found from the reduction of this system of equations are added to the starting values and these new estimates may, in turn, be used as the initial values for the next correction.

The parameters found by all the methods were different only in the number of decimal places of accuracy. Therefore, a listing of the true functions and the approximated functions for comparison is not given.

EXAMPLE II. The set of data for this example was taken from the same function, equation 2.13, but with the random errors added. Success was not as easily, nor as consistently, achieved as with Example I.

The parameters found using only eleven data cards were worthless. They were unpredictable from one set to the next and could not be successfully used as starting values. This was to be expected and after a few such attempts the idea was abandoned.

The "Method of Averages" for finding starting values was only moderately successful. Only one of three sets of initial estimates found was acceptable as starting values.

The method presented in this study produced consistently good results. Almost every set of initial estimates of the parameters were acceptable as starting values. Estimates using 25, 35, and 55 data cards were all acceptable. The smaller number was used thereafter because the program ran much faster.

"Scarborough's Method" was by far the more successful of the two methods for improving the parameters. The "Method of Steepest Descent" was much slower and at times stopped moving the values at all. Apparently, local minima existed in the hypersurface which, with the restrictions imposed, caused the program to exit. Further study to determine better choices of the magnitude of the change in the parameters could possibly make the method more useful.

A summary of the results of a "run" using data from Example II should be worthwhile. Starting values were obtained using 25 data cards. These were improved twice and the data cards were increased to 35. This caused a large increase in the sum of the squares of the residuals but further iterations quickly reduced this sum. It is interesting to note that, using 35 points, the function was more nearly approximating the true data than it was approximating the data being used. An increase to 55 data cards resulted in only a moderate increase in the average error.

For 95 data cards the sum of the squares of the differences between the estimated values and the true values reduced to 1.68, i.e.,

$$\sum_{n=1}^{95}\left[G(x_n, y_n) - ZT\right]^2 = 1.68 \qquad (2.19)$$

whereas the sum of the squares of the residuals had reduced only to 6.43, i.e.,

$$\sum_{n=1}^{95}\left[G(x_n, y_n) - ZE\right]^2 = 6.43. \qquad (2.20)$$

This indicates that the method of least squares produced the desired damping effect.

The list of values from every fifth data point used in estimating the parameters is given in Appendix I for comparison of the responses with errors added, ZE, the true responses, ZT, and the approximations of the responses, ZA.

EXAMPLE III. For the third example parameters were estimated for an approximant to fit a function, equation 2.14, which was not a member of the family of the approximant. The data were "errorless."

Again, starting values were created using 25 data cards and the method presented. The results were excellent from the beginning. To check the ability of the approximant, equation 2.15, to fit the surface throughout the region, R, 95 data cards were ultimately used. The results were

$$\sum_{n=1}^{95} \left[G(x_n, y_n) - ZT \right]^2 = .0076. \tag{2.21}$$

This represents a mean difference between the average error and the true value of the function of .009 which is only 1.6 percent of the value of the mean true value. Apparently the function was a very fortuitous choice.

A listing of every fifth data card is given for comparison of the true responses, ZT, and the approximations of the responses, ZA, in Appendix II.

EXAMPLE IV. The last attempt to determine suitable parameters was made using the data originally taken from the second function, equation 2.12, with random errors added. As had now become regular procedure, starter values were found using 25 data cards. The errors delayed success only a few iterations and increased the sum of the squares of the residuals only slightly. Again, the approximant more nearly fit the true data than the data with errors after 35 data points were included. As in Example II this illustrates excellent damping of the random errors.

Using 95 data cards the results were

$$\sum_{n=1}^{95} \left[G(x_n, y_n) - ZT_n\right]^2 = .028 \tag{2.22}$$

and $$\sum_{n=1}^{95} \left[G(x_n, y_n) - ZE_n\right]^2 = .306. \tag{2.23}$$

The mean error is now .017 or 3 percent of the mean true value. But this is still very good considering the allowable error in the data was 17.2 percent.

A listing of every fifth set of values is given in Appendix III for comparison of the responses with errors added, ZE, the true responses, ZT, and the approximations of the response, ZA.

CHAPTER IV

CONCLUSIONS

Rational polynomials have excellent potential as surface approximants. One of the major disadvantages heretofore was the lack of an adequate method for determining a set of parameters for which one of the criteria of "best fit" could be satisfied. Scarborough's Method appears to overcome this disadvantage by determining "best fit" by the criterion of "least squares" if adequate starting values can be found. The method presented in this study for finding starting values appears sufficiently effective. The study indicates that these two methods used together provide the means necessary for successfully using rational polynomials.

A summary of the procedure found to be most successful is given as follows:

(1) Produce starting values by the method presented using about two data cards per parameter to be found. Twenty-five seemed ideal in the examples in this study.

(2) Start improvements by Scarborough's Method without increasing the number of data points.

(3) When corrections become small increase the number of points. To begin with a large number of points or to increase by too large an amount may cause the corrections to "overshoot" and the solution to diverge.

(4) When an increase in the number of data points does not increase the relative error to a degree beyond

acceptability, a "fit" over the region, R, is indicated.

(5) Iterations for the final number of data cards should be continued as long as a reduction in the sum of the squares of the residuals is significant.

Only by future use for many applications and through further theoretical research will the true value of rational polynomials as surface approximants be known.

There is nothing in the theory discussed that limits the methods presented and discussed to two independent variables. The extension of the methods to any number of independent variables should be obvious.

There is nothing in the theory discussed which limits the rational functions to polynomials. The only limitation necessary is that both the numerator and the denominator be linear in their parameters. Therefore, the use of transcendental terms may be possible.

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APPENDIX I

VALUES FROM EXAMPLE I

X	Y	ZE	ZT	ZA
2.50	.25	.20173394E+01	.16581197E+01	.15247543E+01
1.25	.75	.47151225E+01	.42200000E+01	.44029208E+01
.75	1.00	.50666047E+01	.47804878E+01	.49547123E+01
.25	.50	.42948161E+01	.46666667E+01	.45291360E+01
1.75	1.25	.43272182E+01	.39888889E+01	.40086663E+01
.25	1.25	.37847485E+01	.38333333E+01	.38508707E+01
2.00	1.25	.38943937E+01	.37333333E+01	.37250502E+01
2.00	1.50	.35906144E+01	.38620690E+01	.38324754E+01
1.50	0.00	.13543954E+01	.18461538E+01	.14601571E+01
1.50	.50	.33810361E+01	.33571429E+01	.32802585E+01
1.75	.75	.34137345E+01	.34729730E+01	.34434378E+01
.75	.25	.41910542E+01	.39615385E+01	.39977469E+01
0.00	2.00	.25415089E+01	.22000000E+01	.24168184E+01
3.00	.75	.19511708E+01	.22011834E+01	.22453580E+01
2.75	1.25	.28369178E+01	.30308642E+01	.30440471E+01
2.50	1.75	.30837905E+01	.35757576E+01	.35388374E+01
2.75	1.50	.35088807E+01	.32485549E+01	.32529856E+01
3.00	1.25	.23709392E+01	.28324324E+01	.28780375E+01
2.25	.50	.22126483E+01	.23960396E+01	.22544210E+01

APPENDIX II

VALUES FROM EXAMPLE II

X	Y	ZT	ZA
.25	.50	.11750310E+00	.10562699E+00
1.75	.25	.35435150E+00	.36730453E+00
2.25	1.00	.89460080E+00	.89403075E+00
.75	.25	.17097090E+00	.15566876E+00
1.25	.50	.46473860E+00	.46231942E+00
3.00	0.00	.00000000E-99	-.62291718E-02
1.00	.50	.39346940E+00	.38343406E+00
2.75	1.00	.93607220E+00	.92676198E+00
1.25	.75	.60839440E+00	.60956108E+00
1.00	1.50	.77686990E+00	.77668299E+00
0.00	1.75	.00000000E-99	-.58872274E-02
2.50	.50	.71349520E+00	.71741143E+00
1.00	1.75	.82622610E+00	.81790406E+00
3.00	.50	.77686990E+00	.76039567E+00
1.25	0.00	.00000000E-99	.35392870E-02
1.25	2.00	.91791500E+00	.90029273E+00
2.00	1.00	.86466480E+00	.86673801E+00
.25	1.75	.35435150E+00	.37460472E+00
.50	.25	.11750310E+00	.10284492E+00

APPENDIX III

VALUES FROM EXAMPLE III

X	Y	ZE	ZT	ZA
.25	.50	.49897180E-01	.11750310E+00	.11378238E+00
1.75	.25	.41966289E+00	.35435150E+00	.38771498E+00
2.25	1.00	.87425988E+00	.89460080E+00	.89074186E+00
.75	.25	.88233170E-01	.17097090E+00	.16669466E+00
1.25	.50	.47756413E+00	.46473860E+00	.48599937E+00
3.00	0.00	-.69323658E-01	.00000000E-99	-.22275362E-01
1.00	.50	.43619975E+00	.39346940E+00	.40886789E+00
2.75	1.00	.83826193E+00	.93607220E+00	.92182071E+00
1.25	.75	.57405019E+00	.60839440E+00	.62872925E+00
1.00	1.50	.83324874E+00	.77686990E+00	.78963057E+00
0.00	1.75	.65740784E-01	.00000000E-99	.10251432E-01
2.50	.50	.79202952E+00	.71349520E+00	.72379932E+00
1.00	1.75	.79298391E+00	.82622610E+00	.82973812E+00
3.00	.50	.83127638E+00	.77686990E+00	.76414269E+00
1.25	0.00	-.86903648E-01	.00000000E-99	-.45650051E-02
1.25	2.00	.96031749E+00	.91791500E+00	.90695429E+00
2.00	1.00	.76954671E+00	.86466480E+00	.86573609E+00
.25	1.75	.38688485E+00	.35435150E+00	.41031992E+00
.50	.25	.20137774E+00	.11750310E+00	.10558996E+00

VITA

The author was born on January 30, 1930, at Williford, Arkansas. He received his primary and secondary education between the years 1935-47 from Williford public schools.

He attended Harding College, Searcy, Arkansas, during the years 1949-53 and received a Bachelor of Arts Degree in mathematics.

During the period 1953-57 he taught two years in Missouri high schools, interrupted by two years in the United States Army.

Since that time he has been an instructor in the Department of Mathematics at Missouri School of Mines and Metallurgy. Also, he has been employed each summer at the Rolla Metallurgical Research Center, U. S. Bureau of Mines, Rolla, Missouri.

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