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ESTIMATION OF REGIONAL TRENDS IN GRAVITY USING GRAM ORTHOGONAL POLYNOMIALS

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BY
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A

THESIS

submitted to the faculty of the

UNIVERSITY OF MISSOURI AT ROLLA

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ABSTRACT

A computer program is presented which estimates the trend in a rectangular array of gravity measurements. It is assumed that the regional trend of gravity may be estimated by a low-order polynomial. The method of least-squares is applied to solve for the low-order polynomial which best approximates this trend. Gram orthogonal polynomials are used in the solution of this least-squares surface fit.

The program is tested on a known polynomial and on some hypothetical Bouguer gravity data and found to approximate the regional trend of gravity in these cases.

The importance of eliminating any significant noise in the observations before solving for the polynomial estimate of the trend is emphasized. It is also noted that the residuals need not be normally distributed with a zero mean in order to produce a reasonable approximation to the true residual Bouguer gravity map.

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TABLE OF CONTENTS

		PAGE
LIST OF FIGURES		ii
LIST OF TABLES		iii
I.	INTRODUCTION	1
II.	REVIEW OF THE LITERATURE	3
III.	THE THEORY OF LEAST-SQUARES SURFACE-FITTING BY ORTHOGONAL POLYNOMIALS	6
IV.	AN ANALYSIS OF THE LEAST-SQUARES SURFACE-FITTING COMPUTER PROGRAM	15
V.	A TEST OF THE LEAST-SQUARES SURFACE-FITTING COMPUTER PROGRAM ON A KNOWN POLYNOMIAL	21
VI.	APPLICATIONS OF THE COMPUTER PROGRAM TO SYNTHETIC BOUGUER GRAVITY MAPS	27
	A. Synthetic Bouguer Gravity Map One	27
	B. Synthetic Bouguer Gravity Map Two	33
VII.	THE PROBLEM OF NOISE IN THE SEPARATION OF THE REGIONAL AND RESIDUAL COMPONENTS OF GRAVITY	38
VIII.	CONCLUSIONS	40
	BIBLIOGRAPHY	41
	APPENDIX A- Simplified Flow Chart of the Computer Program	44
	APPENDIX B- The Least Squares Surface-fitting Computer Program	52
	VITA	60

LIST OF FIGURES

Figures Page

1. The Numbering System of the Rectangular Array of Observations 16

2. Form of the Computer Program Output. 19

3. Synthetic Bouguer Gravity Map for Case One 30

4. Residual Bouguer Gravity Map for Case One. 31

5. Computed Residual Bouguer Gravity Map for Case One. 32

6. Synthetic Bouguer Gravity Map for Case Two 35

7. Residual Bouguer Gravity Map for Case Two. 36

8. Computed Residual Bouguer Gravity Map for Case Two. 37

LIST OF TABLES

Tables Page

I. Values of the Polynomial $Z = 1 + x + x^2 + y^2$ 23

II. Mass Distributions Used in the Synthetic Bouguer Gravity Maps 28

I. INTRODUCTION

The measured value of Bouguer gravity at any point may be separated into three different components, namely, the trend or regional component, the residual component, and a random noise component. The trend component is that portion of the recorded gravity caused by deep-seated or broad geologic features. The residual component is that portion of the measured gravity due to anomalous mass distributions which are of interest in geophysical exploration. The noise component refers to any variation of the recorded gravity data from the gravity values which may be properly assigned to either trend or residual effects. Noise can result from observational or instrumental errors, small, near-surface anomalous mass distributions, or other extraneous sources.

The elimination of the trend and noise components from the recorded gravity data produces a residual Bouguer gravity map which is used in all further geophysical interpretation.

It is the purpose of this study to develop a computer program for the Geophysical Observatory of the University of Missouri at Rolla which will effectively eliminate the trend component of gravity while retaining the residual component. Experience has shown that the effects of the trend component may be approximated by a low-order polynomial surface. The method of least-squares is applied to solve for the coefficients of the low-order polynomial which, statistically, best describes the trend present in any given set of data. Orthogonal polynomials are used in the solution of the

coefficients of the approximating function by this method, due to the computational advantages which they afford.

If any significant noise is present in the observations, it must be detected and removed before separating the residual and regional components of gravity, in order to prevent distortion of the residual gravity anomalies.

The computer program is tested on several sets of data to evaluate its effectiveness in eliminating the trend component from the Bouguer gravity map. The results of each of these trials are presented in detail in the following chapters.

II. THE REVIEW OF THE LITERATURE

Griffen (1) was one of the earliest investigators to identify residual gravity and present a technique for separating the residual gravity value at any point from the observed Bouguer gravity value at that point. His method involved the use of a moving mathematical average over each point on the gravity map, as calculated on selected circles about the point in question. Griffen is careful to cite the factors that will affect the resultant residual gravity map when using this method. Nettleton (2) later summarized the work of many authors and enumerated the inconsistencies of various "ring averaging" techniques. Grant (3) discussed regional-residual gravity separation and applied statistical probability to the numerical methods which existed at that time.

Agocs (4) was the first geophysical investigator to apply the method of least-squares to the problem of regional-residual gravity separation. He fitted a plane to a set of gravity observations utilizing the least-squares technique, and suggested that higher order surfaces might be useful in some cases. Simpson (5) fitted low-order, nonorthogonal polynomials to gravitational data by the method of least-squares, using a digital computed in his calculations.

Oldham and Sutherland (6) first recognized the advantage of using orthogonal polynomials in estimating the regional trend of gravity. Their work is based on the

mathematical theory developed by De Lury (7). Grant (8) later extended the ideas presented by Oldham in the most complete article on regional-residual gravity separation by orthogonal polynomials available to date. Although the author was unable to study De Lury's book directly, the pertinent ideas presented by him are restated by both Grant and Oldham. The basic mathematical theory on orthogonal polynomial surface-fitting is covered in detail in Chapter III, The Theory of Least-Squares Surface-Fitting by Orthogonal Polynomials.

Forsythe (9) shows how normalizing the independent variable before calculating the orthogonal polynomials reduces the round-off error produced when performing calculations on a digital computer. Much of the theory of least-squares approximation using orthogonal polynomials is also discussed in his paper.

Ralston (10) has an excellent chapter dealing with least-squares data-fitting techniques in one independent variable in his recent book on numerical analysis. The theory of curve-fitting presented by Ralston is easily extended to surface-fitting with the theory outlined by Grant (8). Ralston meticulously points out the advantages orthogonal polynomials afford in eliminating the need to deal with an ill-conditioned matrix in the calculation of the coefficients of the approximating function by the method of least-squares, and the possible sources of machine-generated errors in calculating these coefficients.

A recurrence relation for generating Gram orthogonal polynomials is derived by Ralston. This recurrence relation is presented in the following chapter. A statistical test, described by Wilks (11), for decisions regarding the degree of the best approximating orthogonal polynomial for a given set of data is also available in Ralston's work.

Clenshaw (12) and Cadwell (13) have written short articles on curve-fitting and surface-fitting, respectively, in recent years. Their articles are useful, primarily, for the analysis of computer time required for different arrays. The mathematical theory is highly condensed and similar to Forsythe's in both cases.

Peikert (14) has developed an IBM system/7090 computer program for least-squares analysis in three dimensions, but it deals primarily with geological data and was not, therefore, extensively studied by the author.

III. THE THEORY OF LEAST-SQUARES SURFACE-FITTING BY ORTHOGONAL POLYNOMIALS

It is convenient to define the Bouguer gravity at any point, (x_i,y_i), by the equation

$$G(x_i,y_i) = Z(x_i,y_i) + R_i + N_i, \qquad (1)$$

where $Z(x_i,y_i)$ is the value of the regional component of gravity at the point (x_i,y_i), R_i is the value of the residual gravity component at the point (x_i,y_i), and N_i is the value of the random noise component at the point (x_i,y_i). It is assumed that the residual gravity components are uncorrelated and, correspondingly, the noise components are uncorrelated. The residuals may exhibit correlation over small, local groups of points, but this correlation is insignificant when the entire set of observations is considered.

The expected value of the noise over the set of observations is assumed to be zero. This assumption should be valid provided a sufficiently large number of data points are analyzed. If, in turn, the expected value of the residual gravity component over the entire set of observations is zero, then defining S_i as

$$S_i = R_i + N_i,$$

it is apparent that

$$E[S_i] = E[R_i] + E[N_i] = 0.$$

This allows equation (1) to be written as

$$G(x_i,y_i) = Z(x_i,y_i) + S_i, \qquad (2)$$

where S_i is the random error which is present in any set of measured data. It is then obvious that

$$E[G(x_i,y_i)\ ] = E[Z(x_i,y_i)\ ].$$

Then, determining a regression surface of the mean of $G(x_i,y_i)$ will specify the regional or trend component of gravity, $Z(x_i,y_i)$, for every point (x_i,y_i).

The assumption of a mean value of zero for the residual component of gravity implies that positive and negative anomalies are equally likely, which, at first, seems highly restrictive. However, small deviations from an expected value of zero for the residual component will alter any regression surface but slightly. On the other hand, large departures from an expected value of zero for the residuals are generally easy to detect on the isogal map of the Bouguer gravity data. Often, the latter case will not require a regional-residual separation for locating the residual gravity anomalies. Thus, the assumption of a mean value of zero for the residuals is not as severe a

constraint as it may first appear.

Let $Z(x_i,y_i)$ be estimated by the function

$$Z(x_i,y_i) = \sum_{k=0}^{m} \sum_{j=0}^{n} b_{kj} \; P_{kj}(x_i,y_i), \qquad (3)$$

where $P_{kj}(x_i,y_i)$ is a set of polynomials of degree k in x and of degree j in y and the b_{kj}'s are undetermined coefficients. One should expect $P_{kj}(x_i,y_i)$ to be restricted to low-order polynomials by the definition of the regional gravity component. Another reason for limiting $P_{kj}(x_i,y_i)$ to low-order polynomials is that the true residual anomalies may be eliminated by fitting the observations too closely.

The method of least-squares calculates the coefficients of the polynomials such that the sum of the squares of the error (residual plus noise) terms is a minimum over the set of observations. Least-squares fitting also allows easy computation of each coefficient, b_{kj}, from the normal equations. Experience has shown that this method possesses excellent smoothing properties which are necessary to preserve the residuals in this case. It is desired, then, to minimize $\sum_i S_i^2$ over the set of observations, or in an equivalent form to minimize

$$\sum_i \left\{ G(x_i,y_i) - \sum_{k=0}^{m} \sum_{j=0}^{n} b_{kj} \; P_{kj}(x_i,y_i) \right\}^2.$$

in order to satisfy this condition it is required that

$$\frac{\partial}{\partial b_{kj}} \left\{ \sum_i [G(x_i,y_i) - \sum_{k=0}^{m} \sum_{j=0}^{n} b_{kj} P_{kj}(x_i,y_i)]^2 \right\} = 0.$$

It is easily verified that the above differentiation results in an expression of

$$b_{kj} = \frac{\sum_i G(x_i,y_i) P_{kj}(x_i,y_i)}{\sum_i P_{kj}^2(x_i,y_i)} \tag{4}$$

for the coefficients of the approximating polynomial.

In matrix notation an equivalent expression is

$$[B] = [P'P]^{-1} [P'] [G], \tag{5}$$

where [P] is the matrix defined as

$$[P] = \begin{bmatrix} P_{00}(x_1,y_1) & P_{01}(x_1,y_1) & \cdots & P_{mn}(x_1,y_1) \\ P_{00}(x_2,y_2) & P_{01}(x_2,y_2) & \cdots & P_{mn}(x_2,y_2) \\ \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \vdots \\ P_{00}(x_i,y_i) & P_{01}(x_i,y_i) & \cdots & P_{mn}(x_i,y_i) \end{bmatrix},$$

[P'] is the transpose of the matrix [P], [G] is the column matrix of the observed gravity value for each point, and [B] is the column matrix of the coefficients for each polynomial. The inverse of the symmetric matrix,

$$[P'P] = \begin{bmatrix} \sum_i P_{00}^2 & \sum_i P_{00}P_{01} & \sum_i P_{00}P_{02} & \cdots & \sum_i P_{00}P_{mn} \\ \sum_i P_{01}P_{00} & \sum_i P_{01}^2 & \sum_i P_{01}P_{02} & \cdots & \sum_i P_{01}P_{mn} \\ \vdots & \vdots & \vdots & & \vdots \\ \sum_i P_{mn}P_{00} & \sum_i P_{mn}P_{01} & \sum_i P_{mn}P_{02} & \cdots & \sum_i P_{mn}^2 \end{bmatrix},$$

where P_{mn} is $P_{mn}(x_i,y_i)$, is required in the calculation of the coefficients of the polynomials by the method of least-squares. Using any arbitrary polynomial will lead to an ill-conditioned matrix which greatly magnifies any round-off error generated in the solution of the least-squares problem. Ill-conditioning refers to a loss of significant figures during calculation by taking the inverse of a matrix whose off-diagonal elements are very large. Fox (15) has a comprehensive discussion of ill-conditioning in his text on numerical analysis.

Churchill (16) defines a particular class of polynomials which satisfy the property

$$\sum_i P_{kj}(x_i,y_i)\, P_{hg}(x_i,y_i) = 0 \qquad \text{if } k\neq h \text{ and } j\neq g, \qquad (6)$$

as orthogonal polynomials. Applying orthogonal polynomials to the solution of the least-squares problem requires that all the nondiagonal elements of the matrix $[P'P]^{-1}$ be zero. Thus, the orthogonal polynomials eliminate, by definition, the need to perform any calculations with an ill-conditioned

matrix in the solution of the least-squares problem. They also shorten computing time and storage space for any given array of gravity data. Another unique advantage of using orthogonal polynomials in this problem is that each coefficient, b_{kj}, is independent, that is, its value is not affected by the degree of the approximating orthogonal polynomial.

Grant (8) shows that if the array of observed gravity data is spaced in equal increments in the x-direction and equal, but possibly different increments in the y-direction, then the orthogonal polynomial $P_{kj}(x_i,y_i)$ may be written as

$$P_{kj}(x_i,y_i) = P_k(x_i)\ P_j(y_i). \tag{7}$$

This allows the orthogonality property to be stated as two separate conditions,

$$\sum_i P_k(x_i)\ P_h(x_i) = 0 \qquad \text{if } k \neq h, \tag{8}$$

and

$$\sum_i P_j(y_i)\ P_g(y_i) = 0 \qquad \text{if } j \neq g. \tag{9}$$

Almost all gravity measurements are taken in such a regular array, and, due to this fact, only data which is spaced in a rectangular array is considered in this study. Methods for dealing with irregularly spaced data are given by Grant.

The question which now arises is what type of orthogonal polynomials to use in the solution of the least-

squares problem. A set of orthogonal polynomials which have been shown to be of great value in the case of equally spaced data are Gram orthogonal polynomials. These polynomials are derived by Ralston (10) for one independent variable and are extended to the two independent variable case with the previously stated theory.

Forsythe (9) found that the round-off error generated in the computation of the coefficients of the Gram orthogonal polynomials was greatly reduced if the independent variable was normalized so that the origin fell in the center of the data set. He defines the normalized independent variable, s, as

$$s = \frac{x - x_0}{h} - L, \qquad (10)$$

where x_0 is the initial value of the independent variable, x, h is the spacing of the observations, and

$$L = (M-1)/2,$$

where M is the number of observations.

Let the coefficients β_j and ϵ_j be defined by the equations

$$\beta_j = \frac{j^2 \left[(2L+1)^2 - j^2 \right]}{4 (4j^2 - 1)} \qquad \text{for } j=1,2,3,\ldots, \qquad (11)$$

and

$$\varepsilon_j = \frac{(2j)!}{(j!)^2} \frac{1}{(2L)\ (2L-1)\ \ldots\ (2L-j+1)} \quad \text{for } j=1,2,3,\ldots, \qquad (12)$$

where (2L+1) is the number of data points under consideration. It can be shown that a three term recurrence relation exists for generating Gram orthogonal polynomials. This relation is

$$P_{j+1}(s,2L)=\varepsilon_{j+1}[s/\varepsilon_j\ P_j(s,2L) - \beta_j/\varepsilon_{j-1}\ P_{j-1}(s,2L)], \qquad (13)$$

where $P_0(s,2L)$ and $P_{-1}(s,2L)$ are defined as

$$P_0(s,2L) = 1$$

and

$$P_{-1}(s,2L) = 0.$$

Then, the value of the orthogonal polynomial at any point is not only a function of the independent normalized variable, s, but also a function of the number of data points in the set of observations, (2L+1).

Letting sx and sy represent the normalized x and y variables, respectively, equation (7) may be written as

$$P_{kj}(sx_i,sy_i) = P_k(sx_i)\ P_j(sy_i), \qquad (14)$$

where $P_k(sx_i)$ and $P_j(sy_i)$ are defined by equation (13) with s replaced by sx and sy, respectively.

The problem which now presents itself is what degree, m (k·j), of the orthogonal polynomial best approximates the

regional component of gravity. If an orthogonal polynomial of some degree, M, exists such that the sum of the squares of the error terms is zero, one should expect the coefficient b_{M+1} and the coefficients of all other higher ordered terms to be zero. Wilks (11) recommends the statistic

$$\sigma^2 = \delta^2/(N-m-1)$$

to test the hypothesis that b_{m+1} equals zero, where

$$\delta^2 = \sum_i S_i^2 ,$$

N is the number of observations, and m is the degree of the orthogonal polynomial being tested. Then, the value of σ^2 should be tested for each degree, m, of the approximating orthogonal polynomial until no significant decrease in its value is noted. The degree, M, of the orthogonal polynomial for which this occurs is then, statistically, the best fit to the observed gravity data. This result is valid if no errors are present in the data or if the errors are normally distributed with a zero mean and some variance σ^2.

A computer program was developed which utilized the method of least-squares in solving for the coefficients of the orthogonal polynomial which, statistically, best approximated the trend in an array of gravity measurements.

IV. AN ANALYSIS OF THE LEAST SQUARES SURFACE-FITTING COMPUTER PROGRAM

A Fortran IV computer program capable of fitting a surface to a rectangular array of up to five hundred data points was written for the Geophysical Observatory of the University of Missouri at Rolla. It is the purpose of this chapter to explain the operation of this program. A flow chart of the program is given in Appendix A and a copy of the program is presented in Appendix B. The program was tested on a known polynomial and on two synthetic Bouguer gravity maps derived from known mass distributions. The IBM system/360 model 40 digital computer of the University of Missouri at Rolla was used in the calculations. The following chapters will present the results of the above tests of the program in detail.

The program was designed to operate on a rectangular array of M data points in the x-direction and N data points in the y-direction. The values of M, N, and the observed Bouguer gravity for each point must be read into the computer for every set of data analyzed. This is the only input that varies for a given set of observations. Each point is assigned a different number from one to I, where I is the product M·N. Figure 1 shows how each point, (x_k,y_k), is numbered. The Bouguer gravity value for each point must be read in sequentially from one to I.

The program assumes that the origin is in the center of the rectangular array of observations and that the

(x_1, y_1) ×	(x_2, y_2) ×	.	.	.	(x_m, y_m) ×
(x_{m+1}, y_{m+1}) ×	(x_{m+2}, y_{m+2}) ×	.	.	.	(x_{2m}, y_{2m}) ×
(x_{2m+1}, y_{2m+1}) ×	(x_{2m+2}, y_{2m+2}) ×	.	.	.	(x_{3m}, y_{3m}) ×
.	.	.	.	.	.
.	.	.	.	.	.
.	.	.	.	.	(x_{jm}, y_{jm}) ×
(x_{jm+1}, y_{jm+1}) ×	(x_{jm+2}, y_{jm+2}) ×				(x_{nm}, y_{nm}) ×

Figure 1

The Numbering System of the Rectangular Array of Observations

grid-spacing is unity in both the x-direction and the y-direction. The first assumption requires that both M and N be odd numbers. The assumption of unit grid-spacing in both directions indicates that the coefficients calculated by the method of least-squares are coefficients of an orthogonal polynomial in the normalized independent variables sx and sy. The latter assumption decreases round-off error in the calculation of the coefficients of the polynomial, Z(sx,sy), which best fits the data, without any loss of generality in the computation of the residual Bouguer gravity at any point.

In order to prevent division by zero in the computation of the coefficients of the orthogonal polynomial which best approximates the regional component of gravity, both M and N must be equal to or greater than seven. It is improbable that one could detect a trend without this condition being satisfied.

The coefficients of all terms up to and including sx^5sy^5 are computed. A trend of this high a degree would, in all likelihood, be geologically impossible by the definition of the regional component of gravity. Thus, by calculating coefficients of terms up to and including this tenth degree term, we are assured of having the coefficients of all the terms necessary for describing the trend in any set of observations if such a trend exists.

The dimensions of the arrays G(I,1) and A(I,36) must be changed in the DIMENSION statement to the number of

observations, I, being analyzed, as matrix subroutines which utilize compact storage are used in the calculation of the coefficients of the orthogonal polynomial that best approximates the regional component of gravity. The FORMAT statement used for reading the Bouguer gravity value of each point may be adapted to suit the data.

The program calculates a constant that approximates the set of observations. In the least-squares sense, this is the best polynomial of zero degree in sx and zero degree in sy for approximating the trend in the gravity data. The statistic

$$\sigma^2 = \delta^2/(N-m-1)$$

and the residual Bouguer gravity value for each point are then calculated using the approximation $P_{00}(sx,sy)$. Then, the coefficients of the terms of the orthogonal polynomial of the next higher degree (first degree in this case) are added to the coefficients of the corresponding terms in the lower degree orthogonal polynomial and the value of σ^2 and each residual value are recalculated. This process is repeated for each orthogonal polynomial, $P_{kj}(sx,sy)$, of degree k in the variable sx and degree j in the variable sy, as k and j range independently over the integral values from zero to five. An illustration of this procedure is given in Figure 2. The program contains no test of the magnitude of σ^2 for purposes of terminating the calculations, as in the final analysis, the selection of the orthogonal polynomial

A set of coefficients for Z(sx,sy) if
$Z(sx,sy) = P_{00}(sx,sy)$.

The value of σ^2 using this estimate of Z(sx,sy).

The value of the residual Bouguer gravity for each point using this approximation of Z(sx,sy).

A set of coefficients for Z(sx,sy) if
$Z(sx,sy) = P_{00}(sx,sy) + P_{01}(sx,sy)$.

The value of σ^2 using this estimate of Z(sx,sy).

The value of the residual Bouguer gravity for each point using this approximation of Z(sx,sy).

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.
.

A set of coefficients for Z(sx,sy) if
$Z(sx,sy) = P_{00}(sx,sy) + P_{01}(sx,sy) + P_{10}(sx,sy) + \ldots + P_{55}(sx,sy)$.

The value of σ^2 using this estimate of Z(sx,sy).

The value of the residual Bouguer gravity for each point using this approximation of Z(sx,sy).

Figure 2

Form of the Computer Program Output

used in estimating the regional component of gravity is a matter of geophysical interpretation. The value of σ^2 and the magnitude of the coefficients of the various terms of the approximating orthogonal polynomial are, of course, important considerations in this interpretation. This is to say that the minimum value of σ^2 does not necessarily correspond to the polynomial which best estimates the regional component of gravity.

The program may be easily revised to analyze more than five hundred points of data by merely altering the DIMENSION statement. This would require, however, more core storage than is currently available on the IBM system/360 digital computer of the University of Missouri at Rolla. It would be necessary to change several statements if one wished to increase the maximum degree of the estimating orthogonal polynomial in order to apply the program to some other problem.

The compilation time of the program when run in G level Fortran IV is two and one half minutes. The total compilation and execution time for various arrays of data are given in later chapters.

V. A TEST OF THE LEAST-SQUARES SURFACE-FITTING COMPUTER PROGRAM ON A KNOWN POLYNOMIAL

In order to measure the accuracy of the coefficients calculated by the least-squares surface-fitting computer program, a known polynomial was evaluated at integral values of its independent variables and these values were read into a digital computer. The polynomial used in this trial was

$$Z = 1 + x + x^2 + y^2.$$

The only purpose of using this particular polynomial was the ease it afforded in the evaluation of $Z(x,y)$ at various integral values of the independent variables. Any polynomial chosen would have served the purpose equally well. Values of the polynomial were calculated at each point, (x,y), as both variables, x and y, ranged independently over the integral values from zero to six.

The computer program is designed to perform all calculations with the normalized x and y variables, sx and sy, respectively. In this case,

$$x = sx + 3$$

and

$$y = sy + 3,$$

since x and y range over the same values. Changing the variables of the original polynomial to sx and sy, the

transformed polynomial is

$$Z = 22 + 7\ sx + 6\ sy + sx^2 + sy^2.$$

Values of the transformed polynomial are given in Table I for $-3 \leq sx \leq 3$ and for $-3 \leq sy \leq 3$. Then, the coefficients calculated by the program should agree with the coefficients of this transformed polynomial.

The statistic σ^2 decreased from a value of $.12782539 \times 10^2$ to a value of $.44811763 \times 10^{-8}$ with the addition of an sx^2 term to the approximating polynomial. Then, the best polynomial approximation, in the least-squares sense, to the data in this case is

$$Z = 21.999939 + 7.0000038\ sx + 6.0000248\ sy + .15764826 \times 10^{-5}\ sxsy + 1.0000029\ sx^2 + 1.0000038\ sy^2.$$

As the maximum value of the sxsy term is $.94588956 \times 10^{-5}$, it may be neglected without a significant loss of accuracy. The residual value at each point using the computed polynomial approximation is zero to at least the third decimal place, indicating that no errors are present in the data, which is indeed the case. Thus, the computed polynomial is in excellent agreement with the actual transformed polynomial. The compilation and execution time required for this array of observations was three minutes and thirty-nine seconds.

TABLE I

VALUES OF THE POLYNOMIAL

$Z = 1 + x + x^2 + y^2$

(x,y) coordinate	(sx,sy) coordinate	z value
0,0	-3,-3	1
0,1	-3,-2	2
0,2	-3,-1	5
0,3	-3,0	10
0,4	-3,1	17
0,5	-3,2	26
0,6	-3,3	37
1,0	-2,-3	3
1,1	-2,-2	4
1,2	-2,-1	7
1,3	-2,0	12
1,4	-2,1	19
1,5	-2,2	28
1,6	-2,3	39

TABLE I (Con't)

VALUES OF THE POLYNOMIAL

$$Z = 1 + x + x^2 + y^2$$

(x,y) coordinate	(sx,sy) coordinate	z value
2,0	-1,-3	7
2,1	-1,-2	8
2,2	-1,-1	11
2,3	-1,0	16
2,4	-1,1	23
2,5	-1,2	32
2,6	-1,3	43
3,0	0,-3	13
3,1	0,-2	14
3,2	0,-1	17
3,3	0,0	22
3,4	0,1	29
3,5	0,2	38
3,6	0,3	49

TABLE I (Con't)

VALUES OF THE POLYNOMIAL

$$Z = 1 + x + x^2 + y^2$$

(x,y) coordinate	(sx,sy) coordinate	z value
4,0	1,-3	21
4,1	1,-2	22
4,2	1,-1	25
4,3	1,0	30
4,4	1,1	37
4,5	1,2	46
4,6	1,3	57
5,0	2,-3	31
5,1	2,-2	32
5,2	2,-1	35
5,3	2,0	40
5,4	2,1	47
5,5	2,2	56
5,6	2,3	67

TABLE I (Con't)

VALUES OF THE POLYNOMIAL

$$Z = 1 + x + x^2 + y^2$$

(x,y) coordinate	(sx,sy) coordinate	z value
6,0	3,-3	43
6,1	3,-2	44
6,2	3,-1	47
6,3	3,0	52
6,4	3,1	59
6,5	3,2	68
6,6	3,3	79

VI. APPLICATIONS OF THE COMPUTER PROGRAM TO SYNTHETIC BOUGUER GRAVITY MAPS

In order to measure the computer program's effectiveness in accurately approximating a regional trend in gravity, synthetic Bouguer gravity maps calculated over known mass distributions were analyzed. These maps were composed of the superposition of the gravitational fields of a large, infinitely long, horizontal cylinder and smaller, spherical mass distributions. The field of the horizontal cylinder is slowly varying when compared to the fields of the smaller, spherical masses. Then, the gravitational field of the horizontal cylinder represents the regional component of gravity and the fields of the spherical masses represent the residual gravity component.

A. SYNTHETIC BOUGUER GRAVITY MAP ONE

The gravitational fields of an infinitely long, horizontal cylinder and two buried spheres were combined into a composite Bouguer gravity map. Values of the contrast density, radius, and depth of burial of each body are given in Table II. The Bouguer gravity map presented in Figure 3 is composed of an array of twenty-five observation points in the x-direction and nineteen observation points in the y-direction. The Bouguer gravity value for each point is accurate to ± .02 milligals. The grid spacing is two hundred feet in both directions. The axis of the horizontal cylinder is superimposed on this figure. Figure 4 is a

Table II

Mass Distributions Used in the Synthetic Bouguer Gravity Maps

Case One			
Body	Contrast Density	Radius	Depth of Burial
horizontal cylinder	0.5	5000'	8000'
sphere	-0.5	300'	1000'
sphere	1.0	200'	500'

Case Two			
Body	Contrast Density	Radius	Depth of Burial
horizontal cylinder	0.5	5000'	8000'
sphere	0.5	300'	1000'
sphere	1.0	200'	500'

residual Bouguer gravity map of the fields of the spherical masses in the absence of the field of the horizontal cylinder. The location of the centers of the two spheres is obvious in this figure. The fields of these spherical masses are masked by that of the horizontal cylinder in the isogal map of the original Bouguer gravity data.

Then, it is the function of the surface-fitting program to approximate the field of the horizontal cylinder and, in so doing, eliminate this calculated field from the Bouguer gravity map to yield a residual Bouguer gravity map which approximates the fields of the spherical masses. The statistic σ^2 decreases from a value of .28591222 to a value of $.32531831 \times 10^{-2}$ when using the polynomial

$$Z = 19.932709 + .50981566E\text{-}02\ sx - .60417354E\text{-}02\ sy + .29440271E\text{-}03\ sxsy - .14422765E\text{-}01\ sx^2 - .31764479E\text{-}03\ sy^2$$

to approximate the regional trend of gravity. This is the first significant decrease in the value of σ^2 and, therefore, this approximating polynomial was used to estimate the trend of the observations. The residual gravity value for each point was calculated using this polynomial. The computed residual Bouguer gravity map is given in Figure 5. This residual map is in excellent agreement with the desired residual map of Figure 4. The true minimum value of the negative anomaly is -.46 milligals. The computed minimum

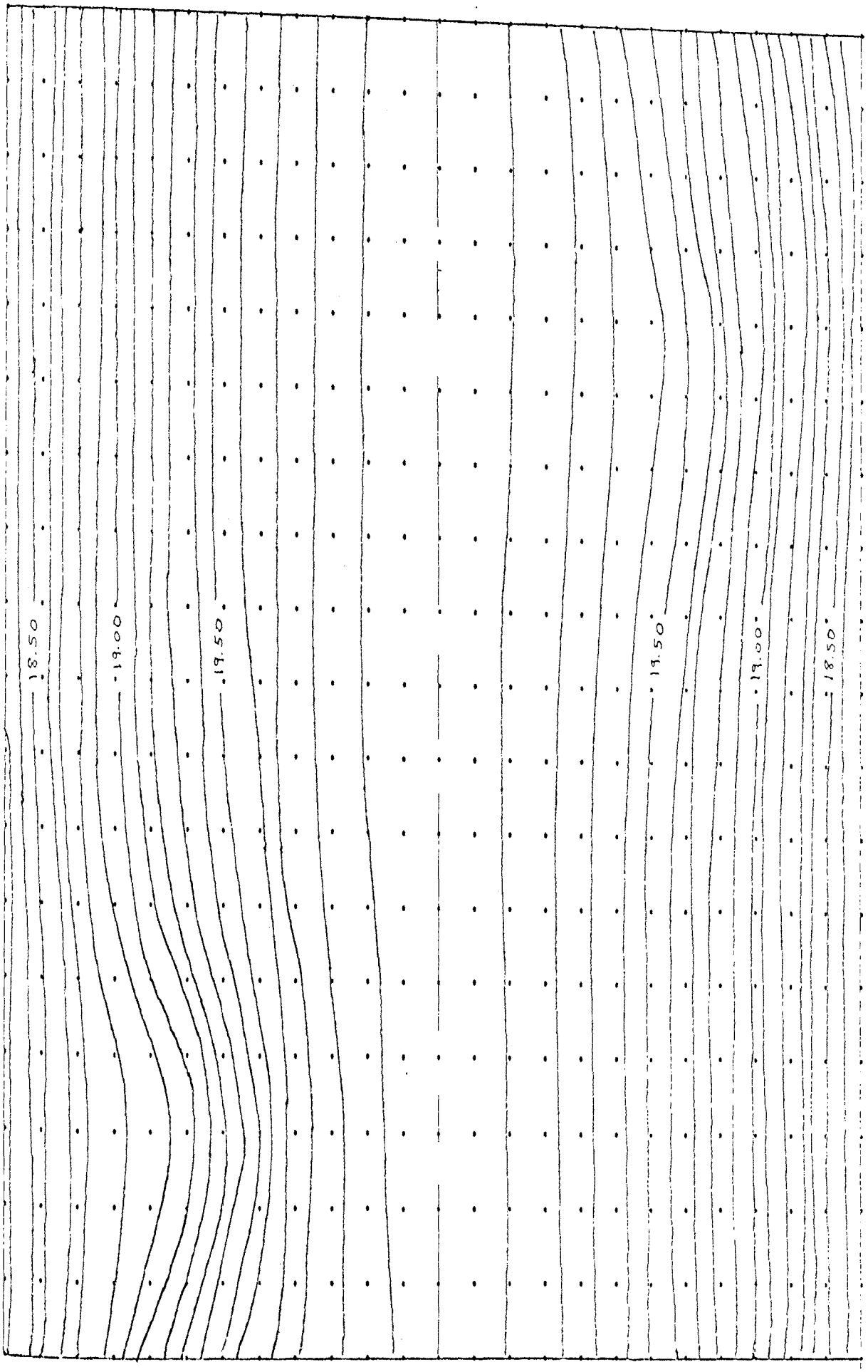


Figure 3

Synthetic Bouguer Gravity Map for Case One

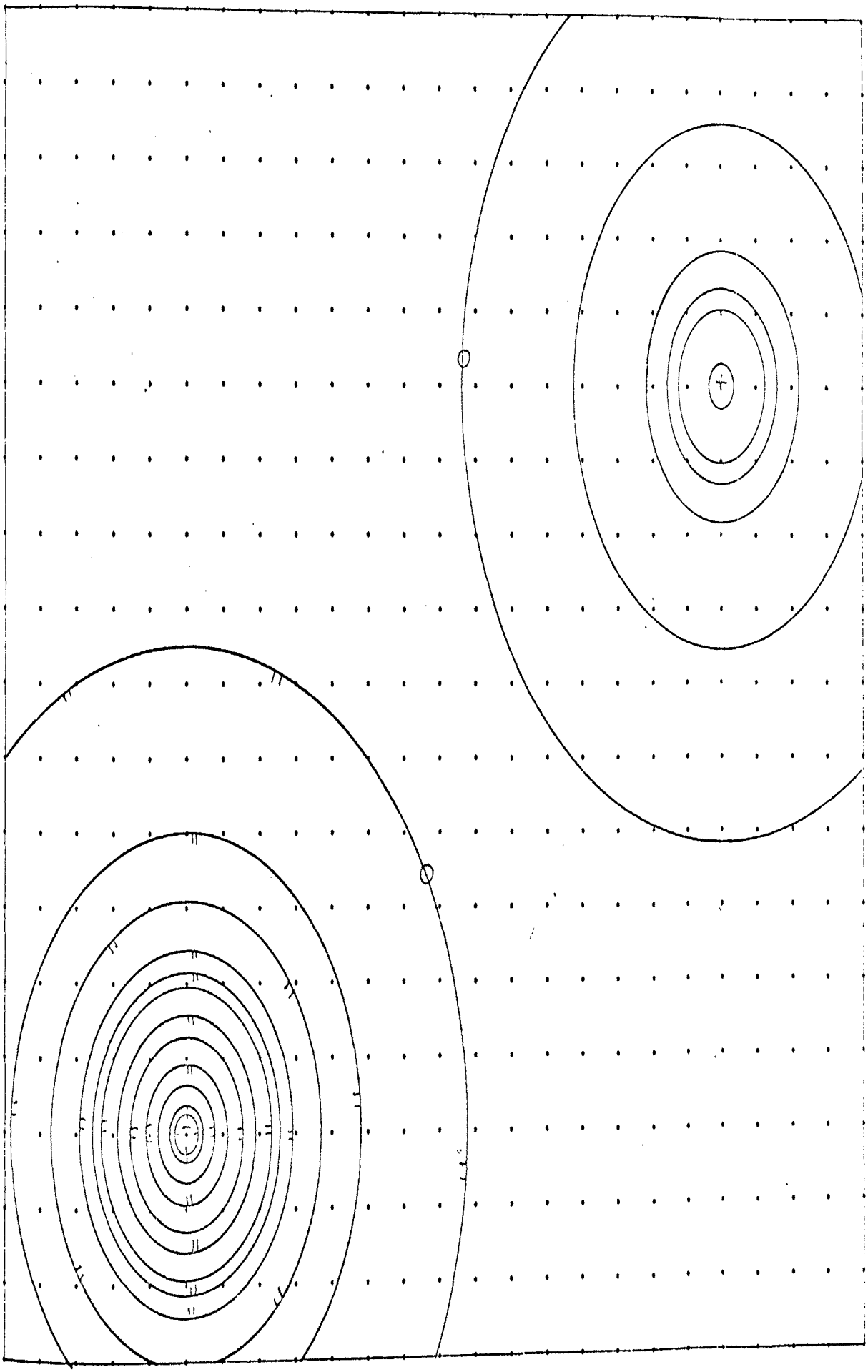


Figure 4

Residual Bouguer Gravity Map for Case One

Figure 5

Legend

x spacing = 200'

y spacing = 200'

contour interval = .04 mgals

value of this anomaly is -.38 milligals. The true maximum value of the positive anomaly is .27 milligals and the computed maximum value is .21 milligals. The minimum value of the negative anomaly and the maximum value of the positive anomaly are coincident on both the computed and the actual residual gravity maps. Distortions of both the amplitude and the areal position of the residual anomalies on the computed residual Bouguer gravity map are due to the fact that the residuals are not normally distributed with a zero mean. It should be noted that even though this condition is not satisfied, the computed residual gravity map is in good agreement with the actual residual gravity map. That is, a reasonable geophysical interpretation of the subsurface may be performed using the computed residual Bouguer gravity map.

B. SYNTHETIC BOUGUER GRAVITY MAP TWO

The values of the contrast density, radius, and depth of burial of the horizontal cylinder and spherical masses used in calculating the second synthetic Bouguer gravity map are given in Table II. These are the same as those used in the first Bouguer gravity map except for the contrast density of the shallower sphere. The isogal map of the Bouguer gravity data is given in Figure 6. The number of observations and the grid spacing are identical to the first gravity map. The Bouguer gravity value for each point is accurate to ±.02 milligals. The true residual Bouguer

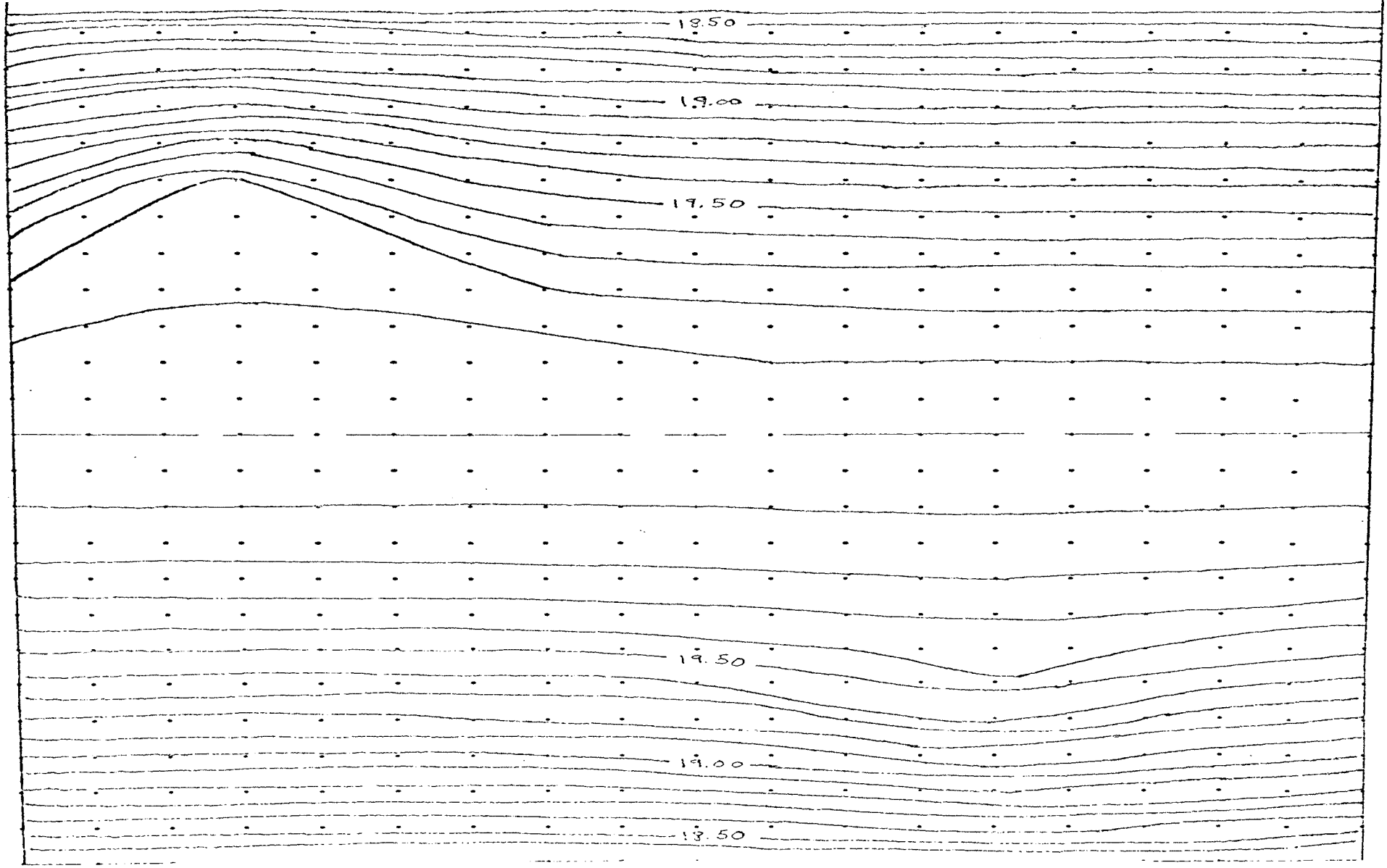
gravity map which is due only to the gravitational fields of the two spheres is presented in Figure 7. The statistic σ^2 decreases from a value of .28515387 to a value of .26339896 x 10^{-2} when using the polynomial

$$Z = 19.970581 - .10610633E\text{-}02\ sx + .25206164E\text{-}02\ sy - .81669074E\text{-}03\ sxsy - .11420067E\text{-}01\ sx^2 - .80105328E\text{-}05\ sy^2$$

to approximate the regional component of gravity. The residual Bouguer gravity map produced using this estimate of the trend is given in Figure 8. The maximum amplitude of the anomaly due to the deeper sphere is .27 milligals. The computed amplitude of this anomaly has a maximum value of .21 milligals. The anomaly due to the shallower sphere has a maximum value of .46 milligals. The computed maximum for this anomaly is .35 milligals. This is in good agreement with the actual residual Bouguer gravity map of Figure 7, even though the departure of the residuals from a zero mean and a normal distribution is greater than in the first synthetic gravity map. The maximum values of both anomalies are again coincident on the two residual Bouguer gravity maps. Thus, the residuals need not be normally distributed with a zero mean in order to derive a reasonably accurate residual Bouguer gravity map.

The compilation and execution time for both maps was eight minutes and fifteen seconds.

Figure 6



Legend

x spacing = 200'

y spacing = 200'

axis of the

horizontal cylinder

contour interval = .1 mals

Figure 7

Legend

x spacing = 200'

y spacing = 200'

contour interval = .04 mgals

Figure 8

Legend

x spacing = 200'

y spacing = 200'

contour interval = .04 mgals

VII. THE PROBLEM OF NOISE IN THE SEPARATION OF THE REGIONAL AND RESIDUAL COMPONENTS OF GRAVITY

Noisy points may distort a residual Bouguer gravity map by introducing false anomalies. Then, it is imperative that any significant noise in the observations be eliminated prior to performing a regional-residual separation of gravity.

Grid-spacings used in conducting any particular gravity survey are selected on the basis of the size and depth of the mass distributions which are of geophysical interest. This means that each residual feature must be detected at several different points in the data set. Then, over small, local groups of points the residuals show correlation. If any noise is present in these observations it will not exhibit this correlation. This is the key to the elimination of the noise from the data set.

It is possible by normalizing a small group of observations and testing each point against a prespecified confidence interval on the normal distribution curve that such noise may be detected. Any noisy point may then be replaced by interpolating a value from the adjacent observations. This process is repeated until the entire set of observations has been tested. With this technique, enough points must be used to insure that the mean and the variance of the group is not greatly influenced by any noisy points. However, the points used with such a technique must exhibit enough correlation of the residuals to insure

that they are not discarded as noise. Satisfying both of these conditions is often not possible, and in such cases the method is not applicable. Some other technique must then be devised for detecting and eliminating the noise. An investigation of different techniques for detecting and eliminating this noise is an excellent subject for further research.

VIII. CONCLUSIONS

The least-squares surface-fitting computer program has been shown to be effective in estimating a regional trend which can be approximated by a low-order polynomial, in a rectangular array of gravity data. The program was shown to fit the trend without greatly distorting any residual gravity anomalies.

The Gram orthogonal polynomials used in the solution of the best polynomial estimate of this trend yielded coefficients which contained no significant round-off errors.

It was seen that the residuals need not be exactly normally distributed with a zero mean in order to obtain a residual Bouguer gravity map which is accurate enough for a reasonable geophysical interpretation of the subsurface.

An analysis of the statistic σ^2 was seen to be sufficient in most cases for selecting the best function for approximating the regional trend of gravity.

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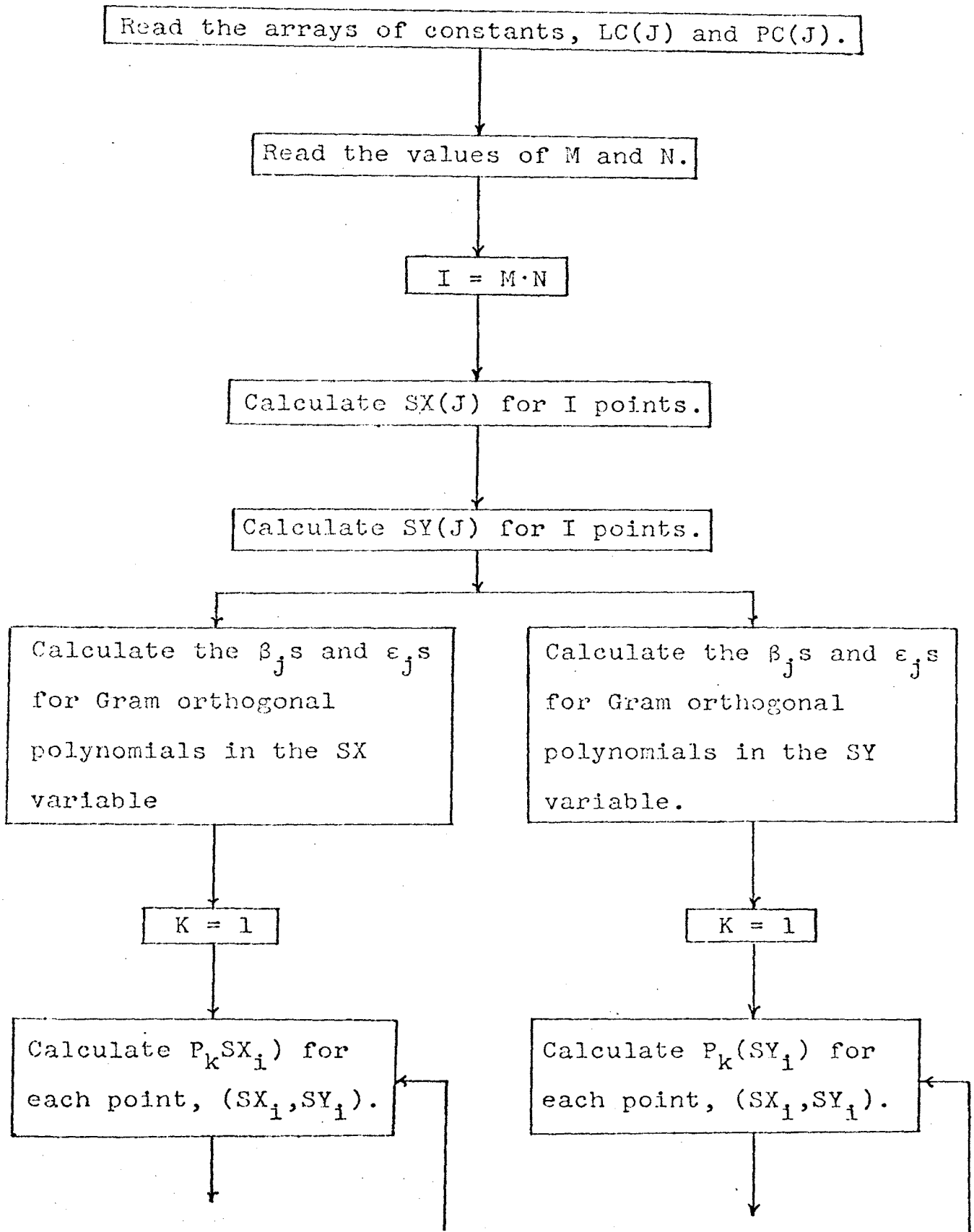
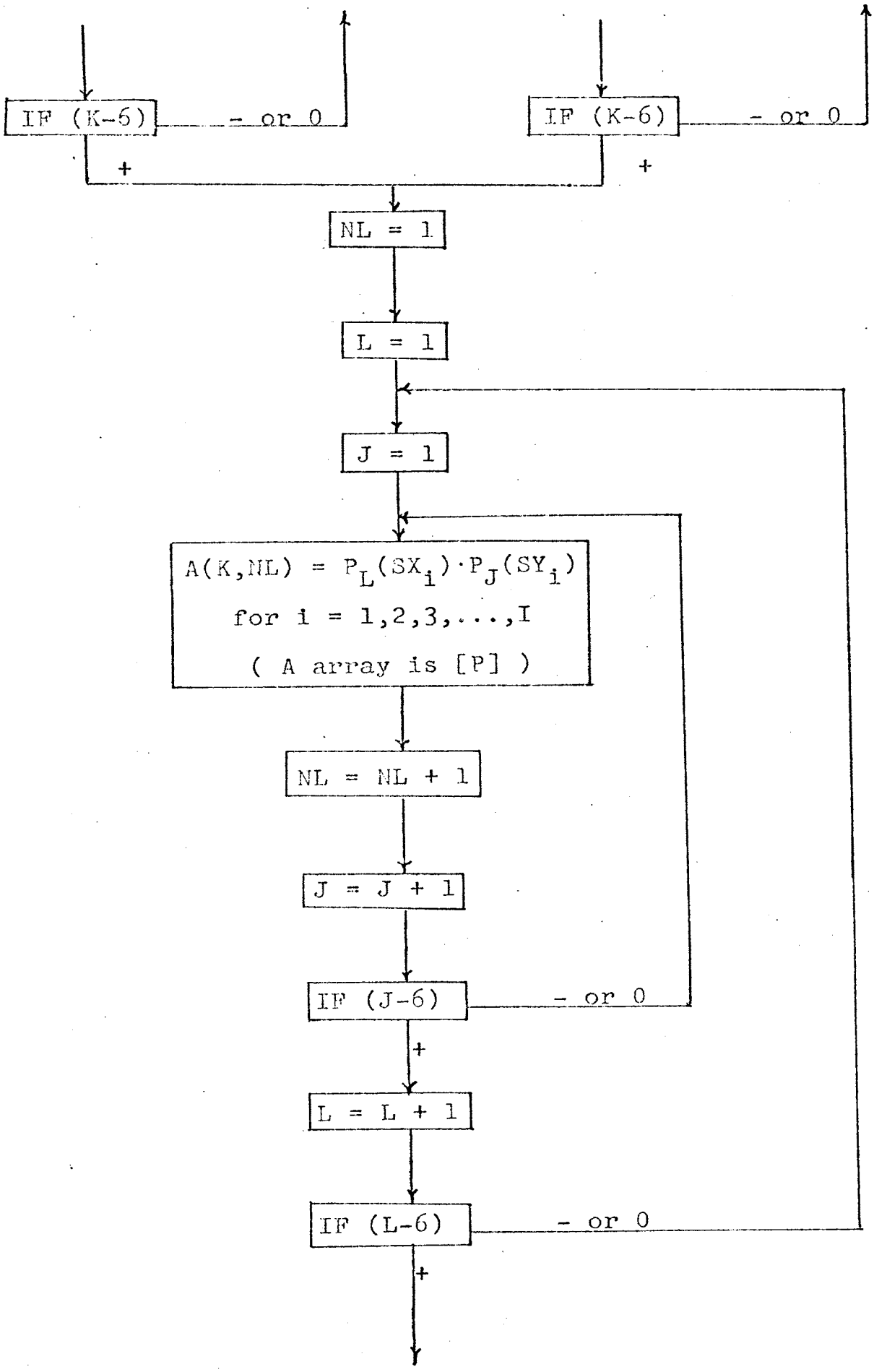
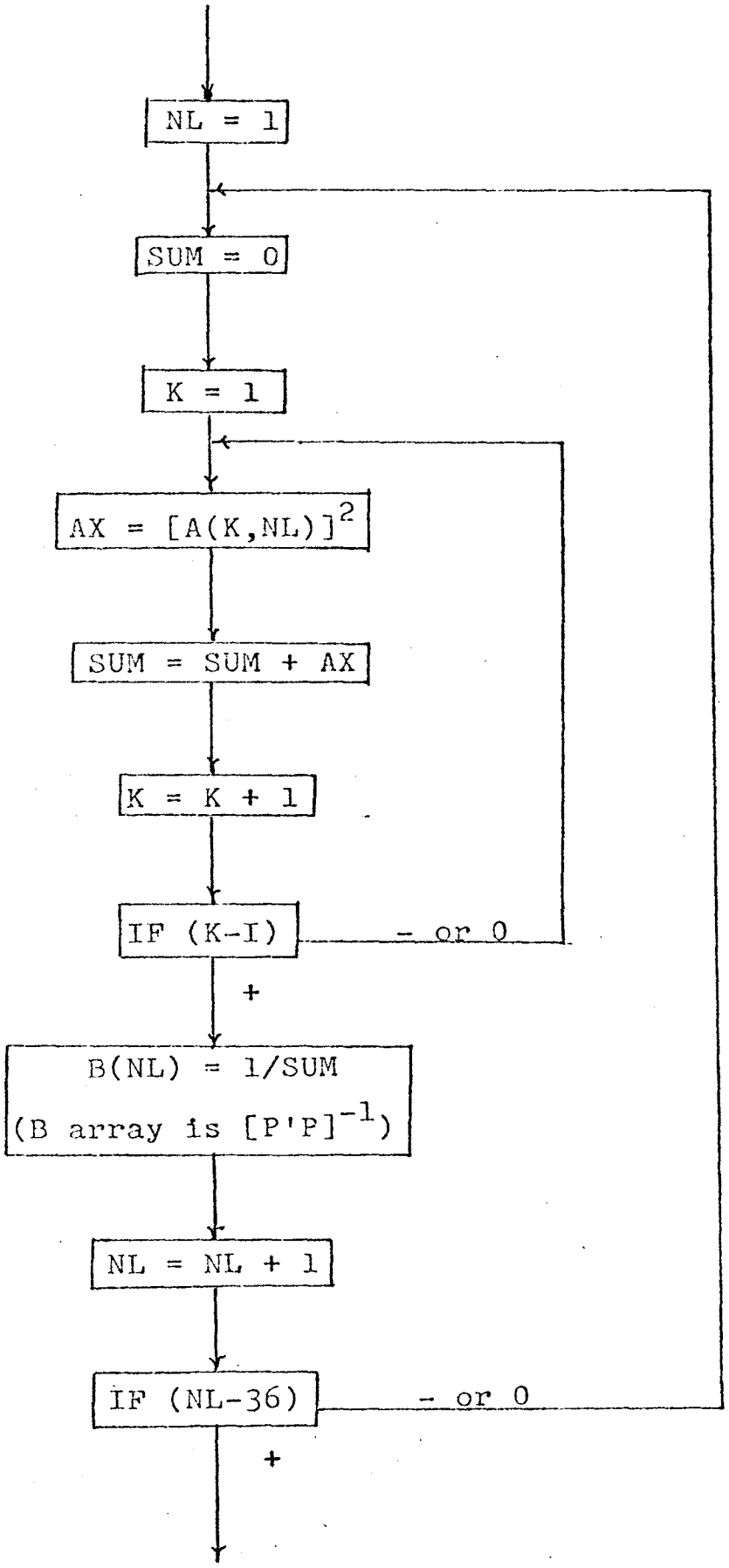
APPENDICES

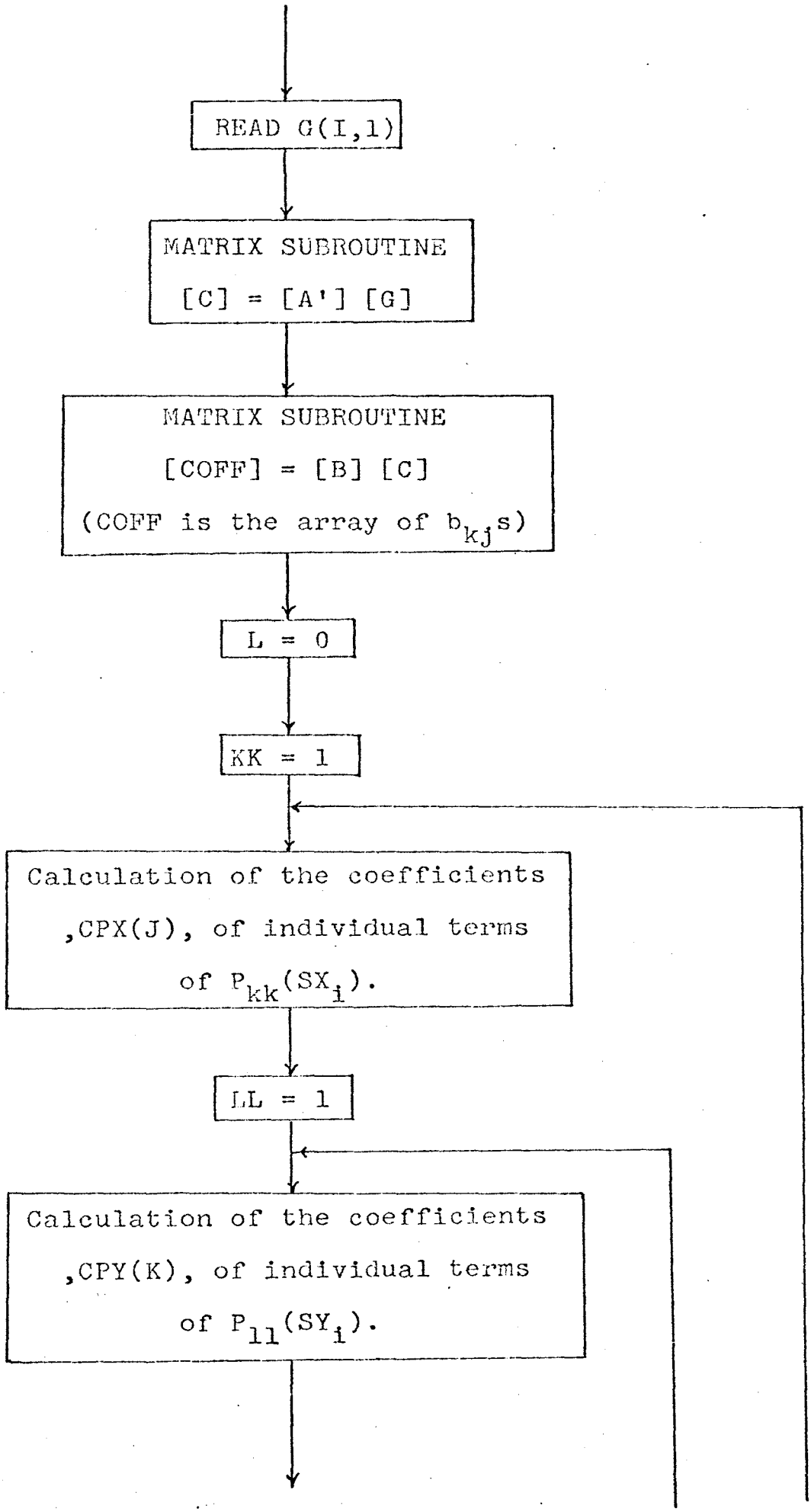
APPENDIX A

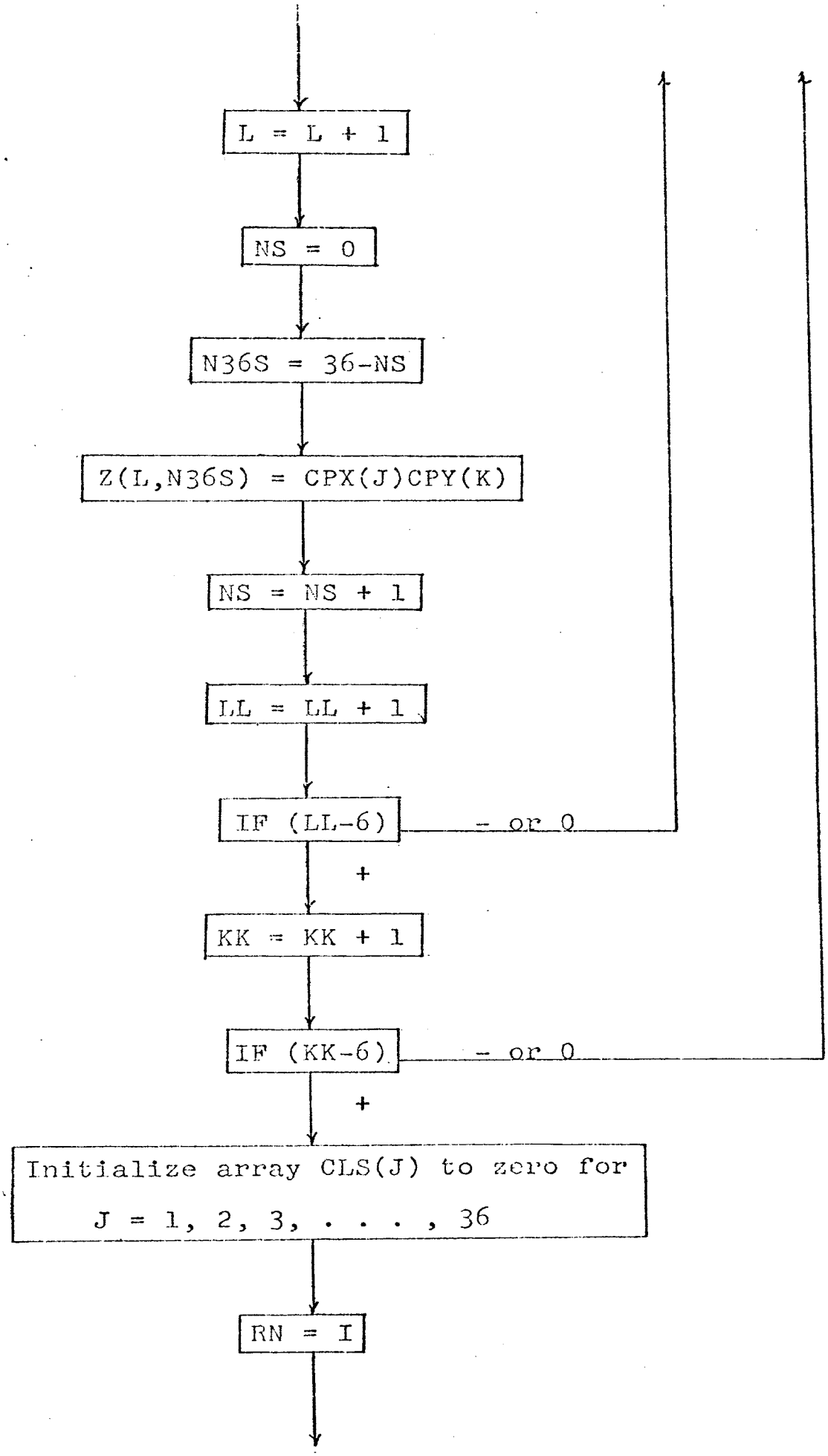
Simplified Flow Chart of the Computer Program

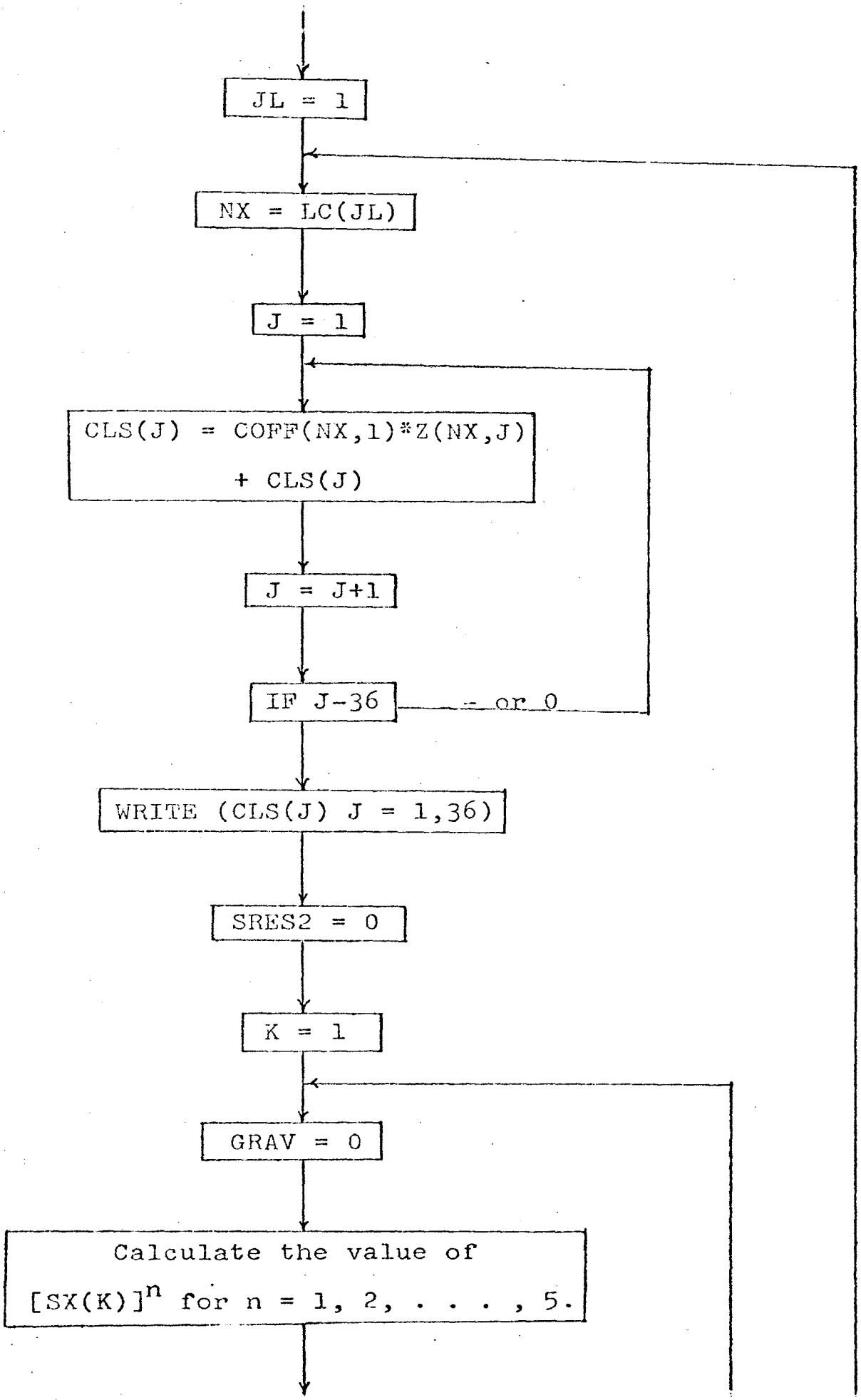


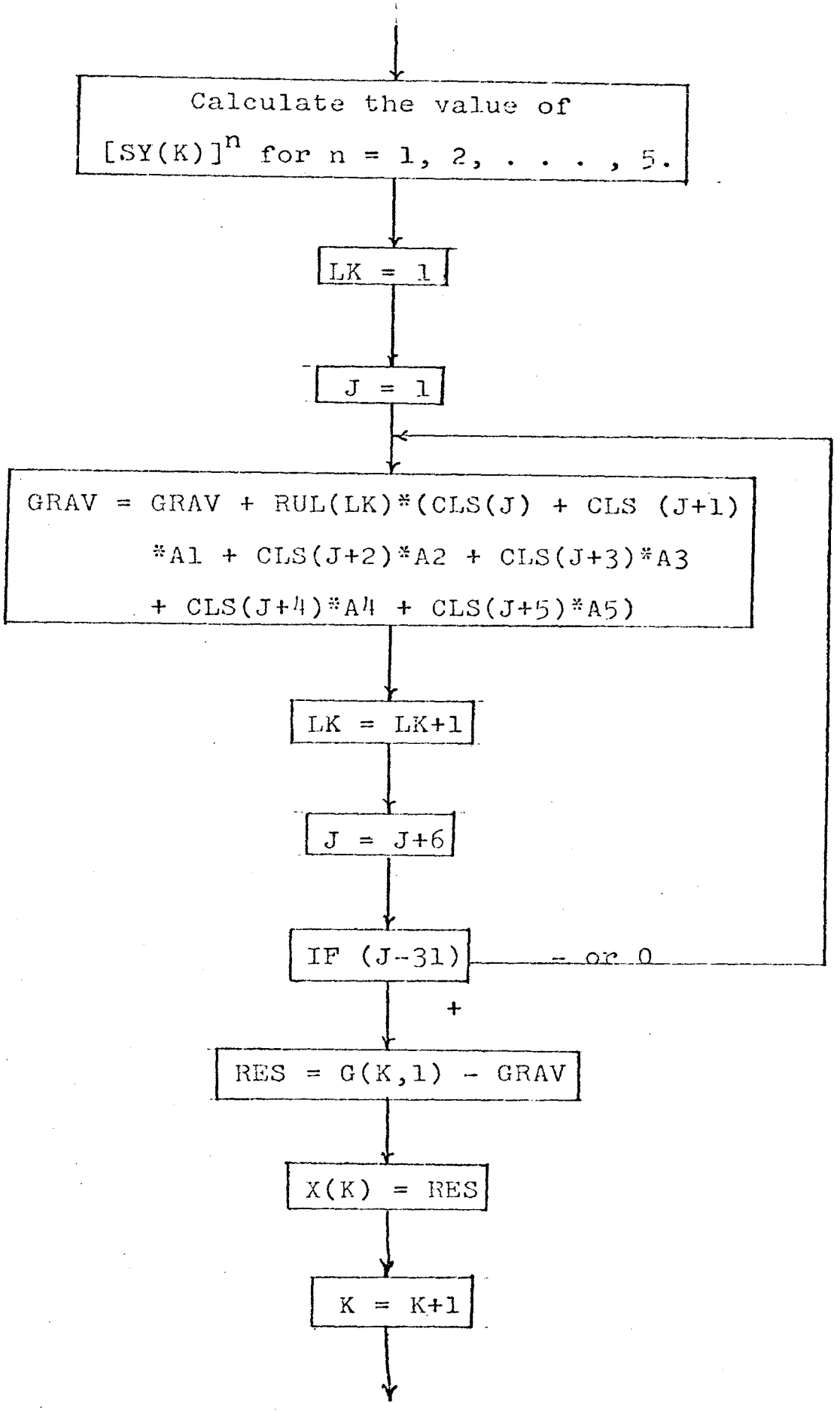

IF (K-6)
- or 0
+
IF (K-6)
- or 0
+
NL = 1
L = 1
J = 1
A(K,NL) = $P_L(SX_i) \cdot P_J(SY_i)$
for i = 1,2,3,...,I
(A array is [P])
NL = NL + 1
J = J + 1
IF (J-6)
- or 0
+
L = L + 1
IF (L-6)
- or 0
+

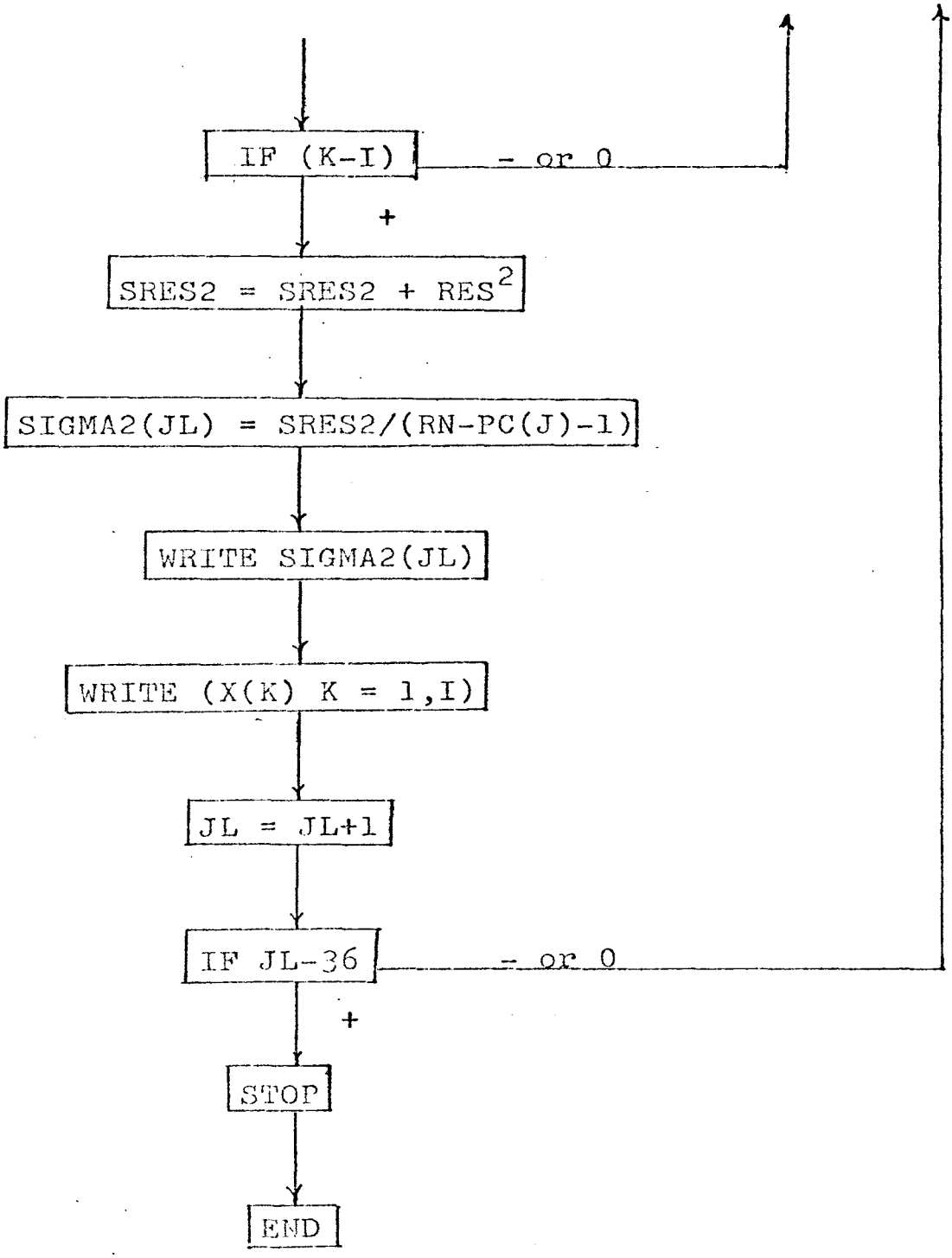

NL = 1
SUM = 0
K = 1
AX = [A(K,NL)]2
SUM = SUM + AX
K = K + 1
IF (K-I)
- or 0
+
B(NL) = 1/SUM
(B array is [P'P]-1)
NL = NL + 1
IF (NL-36)
- or 0
+


READ G(I,1)
MATRIX SUBROUTINE
[C] = [A'] [G]
MATRIX SUBROUTINE
[COFF] = [B] [C]
(COFF is the array of b_{kj}s)
L = 0
KK = 1
Calculation of the coefficients ,CPX(J), of individual terms of $P_{kk}(SX_i)$.
LL = 1
Calculation of the coefficients ,CPY(K), of individual terms of $P_{ll}(SY_i)$.


L = L + 1
NS = 0
N36S = 36-NS
Z(L,N36S) = CPX(J)CPY(K)
NS = NS + 1
LL = LL + 1
IF (LL-6)
- or 0
+
KK = KK + 1
IF (KK-6)
- or 0
+
Initialize array CLS(J) to zero for
J = 1, 2, 3, . . . , 36
RN = I


JL = 1
NX = LC(JL)
J = 1
CLS(J) = COFF(NX,1)*Z(NX,J)
+ CLS(J)
J = J+1
IF J-36
= or 0
WRITE (CLS(J) J = 1,36)
SRES2 = 0
K = 1
GRAV = 0
Calculate the value of
[SX(K)]^n for n = 1, 2, . . . , 5.


Calculate the value of
[SY(K)]^n for n = 1, 2, . . . , 5.
LK = 1
J = 1
GRAV = GRAV + RUL(LK)*(CLS(J) + CLS (J+1)
*A1 + CLS(J+2)*A2 + CLS(J+3)*A3
+ CLS(J+4)*A4 + CLS(J+5)*A5)
LK = LK+1
J = J+6
IF (J-31)
- or 0
+
RES = G(K,1) - GRAV
X(K) = RES
K = K+1


IF (K-I)
- or 0
+
SRES2 = SRES2 + RES^2
SIGMA2(JL) = SRES2/(RN-PC(J)-1)
WRITE SIGMA2(JL)
WRITE (X(K) K = 1,I)
JL = JL+1
IF JL-36
- or 0
+
STOP
END

APPENDIX B

The Least-Squares Surface-Fitting Computer Program

It is the purpose of this Appendix to present a copy of the computer program written specifically for the separation of the regional and residual components of gravity. The program uses the method of least-squares to solve for the coefficients of an orthogonal polynomial which best approximates the trend in a set of observations.

The program requires a rectangular array of observations of M points in the x-direction and N points in the y-direction. The values of M, N, and measured value of each point, G(I,1), are the only input quantities.

```
C     LEAST SQUARES SURFACE FITTING PROGRAM USING ORTHOGONAL
C     POLYNOMIALS.  VALID FOR 500 DATA POINTS
C     VALID TO 5TH DEGREE IN X AND Y.
      DIMENSION X(500),CPY(6),SX(500),SY(500),FMULT(6),FACFX(6),
     1FACFY(6),ETAX(6),ETAY(6),BETAX(6),BETAY(6),POLYSX(7),B(36),
     2PC(36),LC(36),C(36,1),COFF(36,1),Z(36,36),CLS(36),CPX(6),
     3POLYSY(7),RUL(6),SIGMA2(36),G(475,1),A(475,36)
C
      READ (1,109) (LC(J),J=1,36)
      READ (1,120) (PC(J),J=1,36)
C
C     M=NO. OF X DATA PTS., N=NO. OF Y DATA PTS.
C     REQUIRES THAT BOTH M AND N ARE EQUAL TO OR GREATER THAN 7
C
      READ (1,100)M,N
      I=M*N
      READ (1,101) (G(K,1),K=1,I)
      K=1
      L=1
      NN=I+1-M
      MM=M
      XL=(M-1)/2
    2 R=0.0
      DO 1 J=K,MM
      P=R
      R=R+1.
    1 SX(J)=P-XL
      K=L*M+1
      L=L+1
      MM=K+M-1
      IF (K-NN)2,2,3
    3 K=1
      L=1
      YL=(N-1)/2
      T=0.0
      NM=M
    5 P=T
```

```
      DO 4 J=K,NM
    4 SY(J)=P-YL
      T=T+1.
      K=L*M+1
      L=L+1
      NM=K+M-1
      IF (K-NN)5,5,6
C
C     X AND Y VARIABLES ARE NOW KNOWN AND NORMALIZED.
C     CALCULATION OF ETA AND BETA COEFFICIENTS FOLLOWS.
C
    6 P1=1.
      FACT=1.
      FACTN=1.
      P3=1.
      DO 7 J=2,6
      P2=P1+1.
      FACTM=P1*P2
      FACT=FACT*FACTM
      P1=P2+1.
      AFACT=P3*FACTN
      P3=P3+1.
      FACTN=AFACT
    7 FMULT(J)=FACT/(AFACT*AFACT)
      FACX=1.
      FACY=1.
      XLN=2.*XL
      YLN=2.*YL
      R=0.0
      ETAX(1)=1.
      ETAY(1)=1.
      BETAX(1)=0.0
      BETAY(1)=0.0
      BC=(XLN+1.)*(XLN+1.)
      AC=(YLN+1.)*(YLN+1.)
      DO 9 K=2,6
      FACFX(K)=FACX*(XLN-R)
```

```
      FACFY(K)=FACY*(YLN-R)
      R=R+1.
      FACX=FACFX(K)
      FACY=FACFY(K)
      ETAX(K)=FMULT(K)/FACFX(K)
      ETAY(K)=FMULT(K)/FACFY(K)
      PN=(K-1)*(K-1)
      BETAX(K)=PN*(BC-PN)/(4.*(4.*PN-1.))
    9 BETAY(K)=PN*(AC-PN)/(4.*(4.*PN-1.))
C
C       ETA AND BETA COEFFICIENTS NOW KNOWN.
C       EVALUATION OF THE ORTHOGONAL POLYNOMIALS FOR EACH POINT FOLLOWS.
C
      NL=1
      POLYSX(2)=1.
      POLYSY(2)=1.
      DO 20 LN=2,7
      DO 20 LJ=2,7
      DO 29 K=1,I
      IF (LN-2)80,25,23
   23 POLYSX(3)=ETAX(2)*(SX(K)/ETAX(1)*POLYSX(2))
      IF (LN-3)80,25,24
   24 DO 28 J=4,7
   28 POLYSX(J)=ETAX(J-1)*(SX(K)/ETAX(J-2)*POLYSX(J-1)
     1-(BETAX(J-2)/ETAX(J-3)*POLYSX(J-2)))
   25 IF (LJ-2)80,29,26
   26 POLYSY(3)=ETAY(2)*(SY(K)/ETAY(1)*POLYSY(2))
      IF (LJ-3)80,29,27
   27 DO 62 J=4,7
   62 POLYSY(J)=ETAY(J-1)*(SY(K)/ETAY(J-2)*POLYSY(J-1)
     1-(BETAY(J-2)/ETAY(J-3)*POLYSY(J-2)))
   29 A(K,NL)=POLYSX(LN)*POLYSY(LJ)
   20 NL=NL+1
C
C       VALUE OF ORTHOGONAL POLYNOMIALS FOR EACH POINT NOW KNOWN.
C       A ARRAY IS P MATRIX, B ARRAY IS THE INVERSE OF P TRANSPOSE X P
```

```
C       B IS A DIAGONAL MATRIX
C
        DO 22 NL=1,36
        SUM=0.0
        DO 21 K=1,I
        AX=A(K,NL)*A(K,NL)
     21 SUM=SUM+AX
     22 B(NL)=1./SUM
        CALL TPRD (A,G,C,I,36,0,0,1)
        CALL MPRD (B,C,COFF,36,36,2,0,1)
C
C       COFF IS THE ARRAY OF COEFFICIENTS B(J,K) OF THE ORTHOGONAL
C       POLYNOMIALS.  THE EVALUATION OF THE COEFFICIENTS OF THE INDIVIDUAL
C       TERMS IN EACH POLYNOMIAL FOLLOWS.
C
        L=0
        JN=0
        JX=2
        BX=BETAX(2)
        BY=BETAY(2)
        ARX=BETAX(4)*BX
        ARY=BETAY(4)*BY
        DO 40 KK=1,6
        DO 39 J=1,6
     39 CPX(J)=0.0
        J6N=6-JN
        CPX(J6N)=ETAX(JN+1)
        JN=JN+1
        J7N=7-JN
        J9N=9-JN
        IF (JN-3)32,30,30
     30 CPX(J9N)=-CPX(J7N)*BX
        JX=JX+1
        BX=BX+BETAX(JX)
        J11N=11-JN
        IF (JN-5)32,31,31
```

```
   31 CPX(J11N)=CPX(J7N)*ARX
      ARX=ARX+BETAX(5)*(BETAX(2)+BETAX(3))
   32 JY=2
      NJ=0
      DO 40 LL=1,6
      DO 42 J=1,6
   42 CPY(J)=0.0
      N6J=6-NJ
      CPY(N6J)=ETAY(NJ+1)
      NJ=JN+1
      N7J=7-NJ
      N9J=9-NJ
      IF (JN-3)41,34,34
   34 CPY(N9J)=-CPY(N7J)*BY
      JY=JY+1
      BY=BY+BETAY(JY)
      N11J-11-NJ
      IF (NJ-5)41,43,43
   43 CPY(N11J)=CPY(N7J)*ARY
      ARY=ARY+BETAY(5)*(BETAY(2)+BETAY(3))
   41 L=L+1
      NS=0
      DO 50 K=1,6
      DO 50 J=1,6
      N36S=36-NS
      Z(L,N36S)=CPY(K)*CPX(J)
   50 NS=NS+1
   40 CONTINUE
C
C     CLS IS THE ARRAY OF COEFFICIENTS FOR INDIVIDUAL TERMS IN X AND Y
C     AS ADDITIONAL POWERS OF X AND Y ARE ADDED ON INDIVIDUALLY
C     THE VARIANCE OF THE COMPUTED GRAVITY FROM THE OBSERVED GRAVITY
C     IS CALCULATED FOR EVERY ADDITIONAL TERM.
C
      DO 37 J=1,36
   37 CLS(J)=0.0
```

```
      RN=I
      RUL(1)=1.
      DO 72 JL=1,36
      NX=LC(JL)
      DO 38 J=1,36
   38 CLS(J)=COFF(NX,1)*Z(NX,J)+CLS(J)
      WRITE (3,140)
      WRITE  (3,110) (CLS(J),J=1,36)
      SRES2=0.0
      DO 60 K=1,I
      GRAV=0.0
      A1=SX(K)
      A2=SX(K)*A1
      A3=SX(K)*A2
      A4=SX(K)*A3
      A5=SX(K)*A4
      DO 59 J=2,6
   59 RUL(J)=RUL(J-1)*SY(K)
      LK=1
      DO 58 J=1,31,6
      GRAV=GRAV+RUL(LK)*(CLS(J)+CLS(J+1)*A1+CLS(J+2)*A2+CLS(J+3)*A3
     1+CLS(J+4)*A4+CLS(J+5)*A5)
   58 LK=LK+1
      RES=G(K,1)-GRAV
      X(K)=RES
   60 SRES2=SRES2+RES*RES
      SIGMA2(JL)=SRES2/(RN-PC(JL)-1.)
      WRITE (3,111)SIGMA2(JL)
      WRITE (3,130)
      WRITE (3,108) (X(K),K=1,I)
   72 CONTINUE
  100 FORMAT (2I10)
  101 FORMAT (12F6.2)
  108 FORMAT (8F10.3)
  109 FORMAT (18I3)
```

```
110 FORMAT (3X,'Y**0',3X,6E18.8,/,3X,'Y**1',3X,6E18.8,/,3X,'Y**2',3X,
   16E18.8,/,3X,'Y**3',3X,6E18.8,/,3X,'Y**4',3X,6E18.8,/,3X,'Y**5',
   23X,6E18.8,///)
111 FORMAT (/,3X,'VARIANCE =',E18.8,//)
120 FORMAT (12F6.2)
130 FORMAT (3X,'RESIDUAL GRAVITY VALUES AT EACH POINT ARE',//)
140 FORMAT (//,3X,'THE LEAST SQUARES COEFFICIENTS ARE',//,17X,'X**0',
   115X,'X**1',15X,'X**2',15X,'X**3',15X,'X**4',15X,'X**5',//)
 80 STOP
    END
```

VITA

Stanley Dean Thompson was born on August 8, 1944, in Bloomington, Illinois, where he received his elementary and secondary education. He entered the University of Missouri at Rolla in September of 1962 and received the degree of Bachelor of Science in Geophysics from that University in June, 1966. He entered graduate school at the University of Missouri at Rolla in September of 1966 and served as a graduate assistant in the Department of Mining Engineering until the present time.

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