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Linear Inverse Problem in Gravity Profile Interpretation

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Abstract. By an appropriate choice of parameters, the inversion of gravity data can be reduced to a linear system of equations. Generalized inverse theory can be applied to find an optimum solution to the problem provided this is not free and complete. To date, several methods have been published, based either upon least-squares approximations or upon the Backus Gilbert approach. In the present paper, an attempt is made to use other criteria for optimization of the solution, such as linear programming, least-squares and infinite norm approximation. Degeneracy, condition number of the matrix and rounding errors have been considered. A practical problem which severly constrains the data is the size of the system, which depends upon the number of cells used to represent the idealized density model. Several types of cells (rectangular or square prisms and simple polygons) have been tested. Corresponding cell sizes and sample intervals have been compared. Though all the above parameters interact, the norm criterion of the residual is the major factor. In particular, least-squares minimization can lead to drastic effects if not carefully managed, while linear programming leads to more reasonable solutions.

Key words: Gravity – Inverse problem – Norm approximation.

1. Formulation of Problem

The formulaton of what is commonly called the "inverse problem" is very simple and can be reduced to a linear system of equations if some care is taken with the choice of parameters and unknowns. Let

$$\mathbf{b}(b_i,\ i=1,\ m)$$

be a series of measurements of the gravity field in m points; then we have to determine the n parameters.

$$\mathbf{x}(x_j,\ j=1,\ n)$$

which characterize the source of the anomaly, provided that they are related to the data by some kind of relationship A. The formalism of these equations is supposed to be known in order to determine each coefficient constituting

A, i.e.: a_{ij} $(i=1,m;\ j=1,n)$.

The problem is then to solve the system $A \cdot \mathbf{x} = \mathbf{b}$. A solution to the problem can be written as $\mathbf{x}'$ where

$$\mathbf{x}' = \mathbf{x} + \mathbf{e}$$

$\mathbf{e}$ being an random error. In the case of an approximate solution, the problem is to determine $\mathbf{x}'$ with a supplementary condition upon the minimization of the residual $\mathbf{e}$. This last condition generaly depends on a normative definition and can in most cases be adapted to the desired precision upon the solution, provided that it is affected by errors in the data.

The problem can then be written:

$$A \cdot \mathbf{x} = \mathbf{b}$$

and the solution:

$$\mathbf{x}' = \mathbf{x} + \mathbf{e} = H \cdot \mathbf{b}.$$

H is the inverse matrix of A, if it exists, or the generalized inverse in Penrose's (1954) sense.

The interpretation of the above solution has been treated by Lanczos (1961) who defined four types of solution depending upon the relationship between the number of data points m, the number of unknowns n, and the rank r of the matrix A, as follows:

– Free and complete $(m=n=r)$. An exact solution is obtained for any vector $\mathbf{b}$. The inverse H is then the inverse matrix A^{-1} as usually defined. A solution is always obtainable from the computer, though ill-conditioning of the matrix may give rise to a very unstable solution.

– Constrained and complete $(r=n<m)$. This corresponds to an overdetermined set of equations in which $(A^T A)$ is non-singular. The inverse is equal to $(A^T A)^{-1} A^T$ and it corresponds to the least-squares solution in the case of $\mathbf{b}$ being arbitrary. Unfortunately, as Anderssen (1969) pointed out, the normal matrix $(A^T A)$ has a notorious reputation of being ill conditioned; it leads then to very spurious results.

– Free and incomplete $(r=m<n)$. There are less equations than unknowns; the inverse is then $A^T(AA^T)^{-1}$. The solution is not unique and can be regarded as a particular solution, the general solution being obtained by adding a vector deduced from the particular solution, but of rank $n-r$.

– Constrained and incomplete $(r<m,n)$. The solution is not unique: this comes from A being singular if $m=n$, or from $(A^T A)$ being singular if $n<m$. A solution for this case can be found by determining the eigenvectors corresponding to the zero eigenvalues i.e. by solving the system $A\mathbf{x}=0$.

Several papers have been published which take account of the different cases.

A complete and free solution is presented by Emilia and Bodvarsson (1969) through Gauss-Seidel inversion, while discussion has been provided by Bott and Hutton (1970). An incomplete solution is provided through the ideal model of Parker (1975). Numerous applications of the overdetermined system resolution are found in gravity (Braile et al., 1974), resistivity (Inmann et al., 1973) and geomagnetism (Horning et al., 1974). Further papers have provided some sophisticated developments of the above theory (Jackson, 1976; Burkhard and Jackson, 1976).

The purpose of the present paper is to examine the overdetermined case in the light of matrix inversion through different criteria of approximation. In order to compare them, similar data have been tested with each method. Then the model types have been investigated in order to determine the cause of troubles inherent to geometrical parameters.

2. Construction of the A Matrix

It seems obvious that the matrix A will depend upon the type of parameters which are chosen as unknowns. In gravity either geometrical (length and shape) or physical (density contrast) parameters can be chosen. Unfortunately, the first choice leads to non-linear equations which can seriously affect the results on account of instability during inversion; even so, some methods exist which are more or less satisfactory (Corbato, 1965; Johnson, 1969; Dampney, 1969; Inman, 1975). In this paper only a physical parameter (density contrast) will be used, the reason being the reduction of the problems arising during computation; this does not mean, however, total avoidance of them.

The method of construction of the matrix is quite simple. After a choice on how to partition the supposed structure into small cells, the effect of each cell is calculated at each point where the gravity field has been measured. The formula is the now classical one taken from Talwani et al. (1959). However, some modifications are to be taken into account. A simplification can be introduced in the case of a polygon with rectangular cross section (Talwani, 1973). More important is the introduction of a correction for the case of exposed structures. In this case, the formula presents a singularity which arises from numerical division by a factor which tends to zero. A test has been proposed to avoid this problem (Burfeind, 1967).

For a two-dimensional body with polygonal cross section (Fig. 1), the vertical component of gravitational attraction is obtained by calculation of the integral

$$g = 2k\rho \iint_S d\theta\, dr$$

where k is the gravitational constant, ρ the density and S the surface of the source. Since the principles of the method have been given in detail in many review papers and books, the final formula is directly given; the reader may refer for instance to Talwani's (1973) review paper for further reading.

Carrying out the integration for each face of the polygon $(ABC \ldots A)$ and

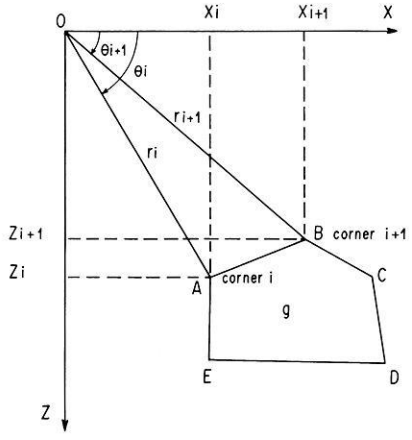


Fig. 1. Gravity effect of the 2-dimensional cell *ABCDEA* at the point 0

summing for all faces the gravity effect of the whole body may be expressed as

$$g(0)=2k\rho\sum_i f_i\cdot\left[(x_{i+1}-x_i)\cdot(\theta_{i+1}-\theta_i)+(z_{i+1}-z_i)\log\frac{r_{i+1}}{r_i}\right]$$

with

$$f_i=\frac{x_i z_{i+1}-x_{i+1}z_i}{(x_{i+1}-x_i)^2+(z_{i+1}-z_i)^2}$$

$$\theta_i=\mathrm{tg}^{-1}\frac{z_i}{x_i}$$

$$r_i^2=x_i^2+z_i^2$$

where x_i, z_i and x_{i+1}, z_{i+1} are the respective coordinates of corners with indices i and $i+1$.

It seems evident that some simplifications can be introduced for the case of a polygon with rectangular corners since the values of either the vertical side or the horizontal one will be equal to zero. The formula reduces then (Talwani, 1973) to

$$g(0)=2k\rho\sum_i(-1)^i\left[z_i\theta_i+x_i\log\left(1+\frac{z_i^2}{x_i^2}\right)\right].$$

In the case of regular cells, an appreciable gain in computation time can be obtained by taking account of the property of symmetry of the attractional field. As each row of the matrix represents the values of the field at different points, it is easy to see that in the case of regular cells with symmetry respect to a vertical axis passing through a point x_k, the values at the points x_{k-1} and x_{k+1} will be the same. If all cells are of the same size and spacing, then it is more advantageous to use the flux density summation method proposed by Jackson

(1975). The time of matrix computation is then reduced by a factor of three, but a disadvantage arises from the attributation of indices, which can easily become complicated.

3. Ambiguity and Non-Uniqueness of the Problem

As far as we are concerned with inverse methods in gravity or in magnetics the major problem remains the non-uniqueness of the results, even in an ideal case without any errors in the data or in the numerical process. This point has been stated a long time ago and Nettleton (1940) wrote that "any mass distribution or geologic condition that is given as a solution for the case of a given gravity distribution depends upon additional controls other than gravity". Some other authors have studied this point. Skeels (1947) has shown that current calculations using sources of simple shapes as usually done with the aid of templates, lead to a wide range of possible structures. Further on, he pointed out that Green's theorem provides an analytical proof of non-uniqueness. Roy (1962) expanded this to other geophysical methods and by means of Green's theorem of the equivalent layer demonstrated the indeterminacy of the solution. Nevertheless, he stated some simple cases in which a solution may be found uniquely. In fact, these cases are the more usual; an example is the density distribution in a single plane at constant depth, or the case where the density contrast is constant and the bounding surface of the source has a known shape. Further, Al-Chalabi (1971) discussed the practical problem and introduced what he called the objective function which is the sum of the squares of the residuals between the observed and computed anomalies. By testing some simple polygons he deduced that a range of values for the density may be obtained for different values of what could be considered as an equivalent radius of the source, but the point is that a correlation does exist between the density and the radius such that all solutions lie within a narrow valley when the objective function is mapped. Naturally, when the number of the parameters increases, so does the ambiguity. This occurs when increasing the number of sides of the polygon. In such a case, several local minima of the objective function develop, but still cluster within the ambiguity valley.

Independent of all this is the non-uniqueness which arises from the computer. In fact, one always obtains a solution from it and that is the trouble. The main point during the calculation is to ensure that the result has some significance. Notwhithstanding which method is used during inversion of the matrix, some problems are to be expected. Two facts are of major importance: conditioning of the matrix and degeneracy.

3.1. Conditioning

The term "condition number" seems to be due to Turing (1948) who defines M and N condition numbers as follows:

$$M(A) = n \max_{ij} |a_{ij}| \max_{ij} |\alpha_{ij}|$$

$$N(A) = n^{-1} \sum_{ij} (a_{ij}^2)^{\frac{1}{2}} \sum_{ij} (\alpha_{ij}^2)^{\frac{1}{2}}$$

(α_{ij}) being the inverse A^{-1} of $A = (a_{ij})$.

Further, Rice defined a theory of conditioning, introducing the condition number $k(A)$ as depending symmetrically on A and A^{-1}, specifically as a product of their norms:

$$k(A) = \|A\| \cdot \|A^{-1}\|.$$

In the case when the spectral or operator norm is used then the spectral condition number $k(A)$ is obtained. In the case of the Euclidean norm, then the so called P-condition number (P = Princeton), is obtained as the ratio of the maximum to minimum eigenvalues.

Some trouble may arise from a matrix with a bad condition number. For instance, for the usual Gauss transformation, it can easily be shown that the condition number is nearly always very large. Let us take the system $A\mathbf{x} = \mathbf{b}$ and using the Gauss method $A^T A\mathbf{x} = A^T\mathbf{b}$, let us look at the spectrum of the matrices $\lambda(A)$, with smallest and largest eigenvalue α and β, respectively, has the spectral range $0 < \alpha \leqq \lambda(A) \leqq \beta$. This leads to $k(A) = \beta/\alpha$. $\lambda(A^T A)$ has a spectral range $0 < \alpha^2 \leqq \lambda(A^T A) \leqq \beta^2$ which leads to $k(A^T A) = \beta^2/\alpha^2$. Then if we have a poor conditioning for the A matrix, i.e. $k(A) = \beta/\alpha \gg 1$ it seems trivial that the condition number of the $A^T A$ matrix will be worse since $k(A^T A) = \beta^2/\alpha^2 \gg \beta/\alpha \gg 1$.

The result is that any iterative process using this type of solution (Tanner, 1967) will converge very slowly even if effective optimization methods are used.

Some devices can be used for having better condition numbers. This can be done through the theory of perturbations and permutations. Different processes may be used in each case by permuting the columns, or by the introduction of a perturbation upon the matrix coefficients by changing the value of the last bit in the computer mode of storing. Some improvements are obtained in this way but they significantly increase the complexity of programming; nevertheless good precision is obtained, even for very bad test matrices (La Porte and Vignes, 1974). An efficient empirical method has been proposed by Mandelbaum (1963). It consists of a reparametrization of the matrix coefficients which has the effect of reducing the length of the spectrum of the matrix, this is done through a translation (change of origin) followed by a homotethy (change of scale).

3.2. Degeneracy

This problem is directly linked to the pseudo-rank of the system of equations. It is evident in the case of overdeterminated systems that there will be some redundancy in the equations. Such a problem, if treated from a theoretical point of view, does not offer major difficulties, but during computation, some trouble may appear mainly because of rounding errors and the incapability of the computer to find exact zero values. Wiggins (1972) has shown that his leads to

the introduction of non-zero eigenvalues. He favoured the use of a cutoff value λ_{lim} in order to ignore all eigenvalues less than this level. This value is determined by examination of the diagram of variances of the resolution vector and the diagram of the solution vector itself; the threshold value provides the effective degree of freedom avoiding numerical instabilities during computation of the pseudo-inverse (Jackson, 1972). The threshold value must be introduced in the algorithm after the examination of each case. In the eigenvalue analysis for the least-squares approximation as proposed by Lawson (1971) and Lawson and Hanson (1974), the eigenvalue spectrum is automatically tapered, avoiding some of the troubles which occur when selecting the cutoff value for the eigenvalue spectrum.

In the same way that the condition number can be tested, degeneracy has to be treated by using perturbations and permutations as far as numerical degeneracy is concerned (La Porte and Vignes, 1974). Round-off errors have been extensively studied by Wilkinson (1963); the reader can refer to this paper for further details.

3.3. Data Accuracy

Random errors due to fluctuations in the data belong to the main difficulties encountered in the inverse problem, when using real data rather than synthetic ones. The errors consist of short wavelength fluctuations. The case has been treated by Bott and Hutton (1970) for the magnetic data inversion. This short wavelength instability is related to the ratio D/W where D is the depth of the source and W the width of the block; this ratio must be choosen as small as possible but in any case it can not exceed 3, a good value is between 1 and 2.

Long wavelength instability occurs because of the finite extent of the data. This results in values at the end of the profile which are non zero; then the inversion tends to place the source at the deepest part of the structure. (This comes from the equivalent layer theorem). The difficulty can be removed by specifying the values of the density contrast at the end of the profile or by extension of the data with some smoothing or apodization. In that sense, a long-wavelength instability exists. It does not correspond to the definition proposed by Bott (1973) who considered only the instability due to a uniform horizontal layer of constant density.

4. Methods of Solution

The use of the least-squares approximation is very common in the case of more data than unknown. Two major objections may be raised against such a use; first, the least-squares function is not strictly convex, and some care must be taken before using it for a large set of data representing more than one anomaly; second, the least-squares method is sensitive to very out-of-range data. This last point has been shown by Claerbout and Muir (1973) with emphasis on the absolute-value norm minimization. In fact, there are other norms existing in the

specialized literature; but for reasons of clarity and time, only three norms have been examined in this paper: these are the so-called l_1 norm, i.e. the sum of the absolute values of the residuals, the l_2 norm or least-squares norm, i.e. the sum of the squared residuals, and the l_∞ norm or Chebyshev norm which is defined as

$$\lim_{p\to\infty} \left|\sum_m (A\mathbf{x}-\mathbf{b}-\mathbf{r})^p\right|^{1/p}.$$

The definitions represent the median, the mean and the mid range respectively (Claerbout and Muir, 1973). Their respective advantages will be compared with synthetic cases. From a computational point of view, these three methods are tested using different programs offered in the available literature.

4.1. l_1 Norm Approximation

The concept of what may be called "least first power" approximations is not yet familiar to the experimental scientist, though there are now several algorithms; some reasons may be advanced. The approximating functions used by experimentalists are almost never polynomials and they rarely constitute Haar sets[1]; few statistical tests are available for the absolute value norm. Nevertheless, l_1 approximations are often superior to l_2 approximations and if the data contain some inaccurate points, no good representations are to be expected from the l_2 norm, but they may be expected from the l_1 norm (Barrodale and Young, 1966).

Barrodale and Roberts (1973, 1974) have provided an algorithm for linear approximation on discrete sets derived from the simplex algorithm. The problem is to minimize the quantity

$$\mathbf{e}=\mathbf{b}-A\mathbf{x}.$$

One way is to decompose the residual vector into the sum of two vectors, each one being non-negative.

$$\mathbf{e}=\mathbf{e}^+-\mathbf{e}^-$$

In the same way x may be decomposed into two parts, both being non-negative:

$$\mathbf{x}=\mathbf{x}^+-\mathbf{x}^-$$

Then the problem is to minimize the sum

$$\sum_i (e_i^+ + e_i^-)$$

subject to $\mathbf{b}=\mathbf{A}(\mathbf{x}^+-\mathbf{x}^-)+\mathbf{e}^+-\mathbf{e}^-$. Since all components of the vectors $\mathbf{x}^+$, $\mathbf{x}^-$, $\mathbf{e}^+$, $\mathbf{e}^-$, are non-negative with this method, a simplex algorithm can be applied.

[1] A set of n continuous functions u_i is called a Haar system provided the number of zeros of $\sum_{i=1}^{n} a_i u_i$ is at most $n-1$ for every choice of the n coefficients a_i

A major problem has been solved with respect to the occasionally time consuming algorithm for the simplex method: it consist of passing through several neighboring simplex vertices in a single iteration (Barrodale and Roberts, 1973).

Time consumption which was the major drawback of the linear l_1 minimization has since been resolved; it was formerly of the order of n squared (where n is the greater dimension of the coefficient matrix); it is considerably reduced and is now quite comparable to that of other methods. In practice, the total number of iterations is close to the smaller dimension of the coefficient matrix. This reduction offers some advantage over the method presented by Claerbout and Muir (1973) which is of the n squared type with regard to time consumption.

4.2. l_2 Norm Approximation

A great number of methods are available for the so-called least-squares approximation. Since some problems arising from ill conditioning have been presented earlier, the method chosen is adapted from Penrose's (1954) decomposition. Given A, an $m \times n$ matrix, there exist three other matrices U, S and V such that $A = USV^T$ where U and V are square orthonormal matrices of order m and n respectively. The S matrix is a diagonal matrix whose elements are the eigenvalues of A; it consists of k numbers different from zero, k being the rank of matrix A. Thus the linear system $A\mathbf{x} = \mathbf{b}$ can be transformed into $S\mathbf{p} = \mathbf{g}$ where $\mathbf{x} = V\mathbf{p}$ and $\mathbf{b} = U\mathbf{g}$. The U matrix can be constructed by taking the eigenvectors associated with the columns of A, and V by taking the eigenvectors associated with the rows of A. An important application is the construction of two matrices associated with U and V, which can be defined as $R = VV^T$ and $Q = UU^T$. Backus and Gilbert (1968) have shown that for an under-determined system, the R matrix represents a measure of the resolution which can be obtained from the data. Similarly, for overconstrained systems, Q represents a measure of the information given by the corresponding observation to the solution. A review of the eigenvalue decomposition of a matrix is given by Golub and Kahan (1965). It includes a bibliography dealing with applications and algorithms. More recently, a detailed book has been issued on the subject (Lawson and Hanson, 1974); it contains nearly everything concerning the theorems and the practical applications of the algorithms.

Two major points are to be expected from the matrix decomposition. It allows a certain degree of uncertainty in the data which can be used to modify the decomposition. Let us take a value e, then each eigenvalue can be modified by less than this value e so that each modified eigenvalue is either zero or greater than e. The condition for that is to take the value e as the upper bound of the spectral norm of uncertainty dA. This can be used for stabilizing the solution of the linear system if it is too badly conditioned.

Another main point is the analysis of the eigenvalue decomposition. This has been examined in detail by Wiggins (1972) and Jackson (1972). It concerns the relationship existing between the rank of the matrix and the modulus of the eigenvalues. Jackson (1972) pointed out the systematic trade-off between re-

solution and variance in the estimation of the successive unknown parameters. As a rule, he proposed a cut-off value for the eigenvalues below which the calculated variance of the parameters was too high and then had no significance. When plotting the successive eigenvalues, one can see from the shape of the curve where the cut-off value is to be taken. A more precise way to do it is to plot the respective norm of the residual vector versus the norm of the solution vector, this norm stabilizes while the norm of the solution vector grows very drastically. The "true" value for the solution is then the one for which both norms are minimum (Fig. 2). This can be interpreted as follows. For an $m \times n$ overdetermined system, there exist n solutions. It is trivial that the solution with the n parameters equal to zero is included. For the same reason, one can easily find a solution vector where all the components are tending towards infinity (negative or positive). When plotting the n solutions on the same diagram, one can see a trend of the respective unknown parameters to tend towards a stabilized solution, then to diverge rapidly. The "good" solution is situated in the portion of the diagram where all solutions do not vary too drastically, while the residual norm tends to zero (Fig. 3).

An improvement to the cut-off value proposed by Wiggins (1972) is feasible by using some device in order to avoid the eigenvalues becoming very small. This can be done through tapering the eigenvalue spectrum by means of what has been called "damped least-squares". Classical least-squares are defined as the minimization of $\mathbf{e}=(A\mathbf{x}-\mathbf{b})^T\ (A\mathbf{x}-\mathbf{b})$ for the parameters $\mathbf{x}$. This involves the computation of the normal equation $A^TA\mathbf{x}=A^T\mathbf{b}$ and then the inversion $\mathbf{x}=(A^TA)^{-1}A^T\mathbf{b}$. In practice, this is done by the matrix decomposition suggested by Lanczos (1961)

$$A=USV^T \quad \text{and} \quad \mathbf{x}=(VS^{-1}U^T)\mathbf{b}.$$

The matrix S is a diagonal matrix containing the eigenvalues of the normal matrix A^TA. Then, S^{-1} will still be a diagonal matrix, but containing the inverse of the eigenvalues $1/\lambda$.

From studies on non-linear least-squares, Marquardt (1963) proposed a damping for the method. The idea had already been offered by Levenberg (1944), and a combination of both has led to the socalled "ridge regression" or Levenberg-Marquardt algorithm, see Marquardt (1970). The technique consists in minimization of the quantity

$$elm=(A\mathbf{x}-\mathbf{b})^T(A\mathbf{x}-\mathbf{b})+\theta^2\mathbf{x}^T\mathbf{x}$$

with θ a weighting coefficient which can in a more general way be replaced by a weighting matrix whose coefficients are the inverse variance and covariance of the estimated parameters. Computing the normal equations leads to

$$(A^TA+\theta^2 I)\mathbf{x}=A^T\mathbf{b}.$$

I being the identity matrix; the generalized inverse is then

$$H=(A^TA+\theta^2 I)^{-1}A^T.$$

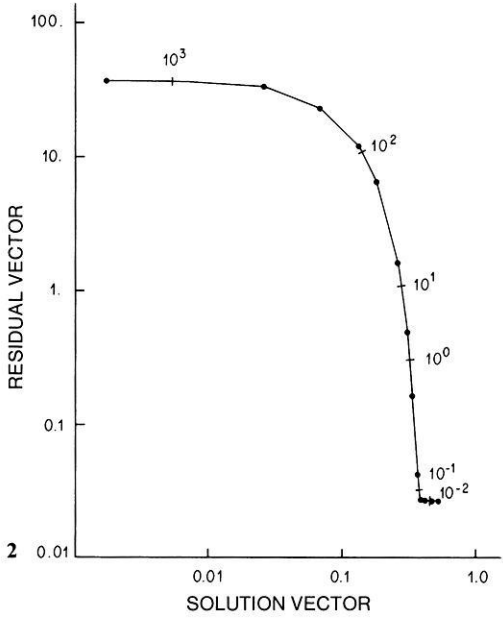
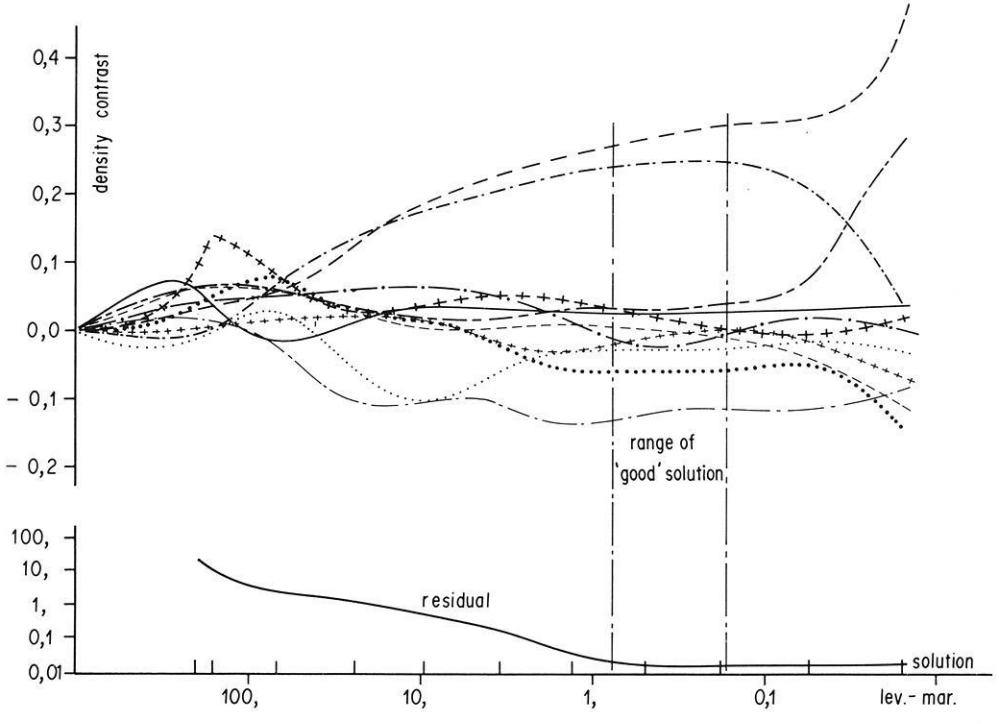


Fig. 2. Norm of residual vector versus of solution vector. Successive black dots represent candidate solution. Line indicates the corresponding value of the Levenberg-Marquardt parameter decreasing all along the curve

Fig. 3. Solution coefficients and residual norm versus Levenberg-Marquardt (LM) parameter. System to solve had 11 unknowns. The different values of each of them have been calculated for different values of LM parameter. The flat part of all curves (for LM parameter value between 0.8 and 0.08) is the range of "good" solutions. The residual is small enough while the variance of the solution is mini um. Solution corresponds to all values equal to zero, except two equal to 0.25



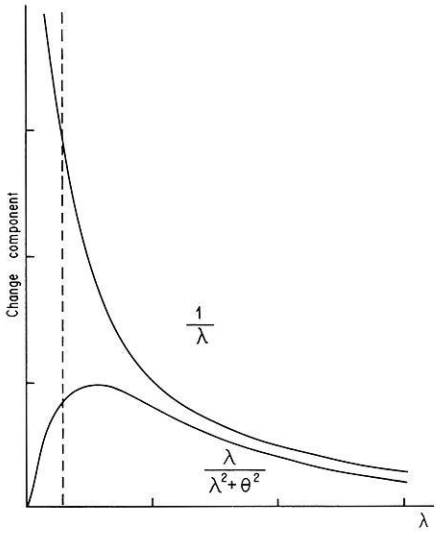


Fig. 4. Representation of the change component in the eigenvalue spectrum when using classical least squares ($1/\lambda$) and damped least squares ($\lambda/(\lambda^2+\theta^2)$). The cutoff value of Wiggins (1972) is indicated as a broken line

Practical computation is done through the matrix decomposition

$$A = USV^T$$

$$\mathbf{x} = V(S^2+\theta^2 I)SU^T\mathbf{b}$$

which can be written

$$\mathbf{x} = VMU^T\mathbf{b}.$$

M is then a diagonal matrix with the quantities $\lambda/(\lambda^2+\theta^2)$ as coefficients.

The change component in the eigenvalue spectrum is then tapered. The difference between classical least-squares and Levenverg-Marquardt is shown in Figure 4.

The use of this last algorithm is of interest because it avoids examination of the eigenvalue spectrum and the cut-off value determination as proposed by Wiggins (1972). Tapering introduced by the θ coefficient stabilizes the pseudo-inverse computation as well. For a special analysis, it can be useful to plot the norm of the residual vector and the norm of the solution vector versus the Levenberg-Marquardt coefficient. Then one can easily see the effect of its lowering until the candidate solutions stabilise.

From a computational point of view, several types of algorithms have been offered in the literature. Most usual is decomposition through the eigenvalues and eigenvectors (Penrose, 1954). This can be done with usual routines, plotting the diagram of the resolution and the respective variance and then calculating the 'best' solution. An improved version is given in Lawson and Hanson (1974). It basically uses the QR decomposition. Another algorithm, a little shorter, is given by Golub and Businger (1965) using the Householder transformations[2]. Some

[2] Householder transformations reduce the matrix to upper right triangular form by means of successive orthogonal transformations

further improvements to the methods are of interest; one consists in the introduction of supplementary constraints on the solutions, a more simple one being positivity of the solution which can be easily reversed to non-positivity if necessary. Of greater use is the possibility of deleting some variables; this can be of great interest in geophysics when other data, of geological type for instance, are provided.

4.3. l_∞ Norm Approximation

For some unknown reason the infinite norm criterion, giving Chebyshev or minimax solutions to an overdetermined system of linear equations, is not popular within the scientific community. One may argue that the midpoint solution bisects the distance between the extreme data points and thus leads to an erroneous solution if some errors are included in the data. It seems, however, in some cases cases interesting to take account of that property, for example in the case of a sharp peak in the data caused by a local structure with strong density contrasts. From a computational point of view, a numerical method for Chebyshev solutions is directly obtainable from a modified simplex algorithm. Stiefel (1959) provided the so-called exchange algorithm, using Jordan elimination in a technique derived from the simplex method. This type of solving linear equations is computationally unstable. It is therefore preferable to use the more stable *LU* decomposition as done by Bartels and Golub (1968). In quite a similar way, Barrodale and Phillips (1974) presented an improved algorithm using the exchange method, but it differs from the previous one in the sense that no restrictions are imposed upon the given function minimizing the residual, and also convergence is accelerated because of the automatic construction of an initial approximation very close to the final solution.

The method of minimax solutions is based on an iterative process which is supposed to converge towards the solution. As in all these methods, the algorithm fails when two or more solutions are close together or when the slope of the hyperplane is such that convergence is not obtainable through a manageable number of iterations. Unfortunately, no solution to these two problems is available at the moment.

The main principle used in the l_∞ approximation problem is to determine an approximate value of the function such that the quantity

$$\text{Max}\,|\mathbf{e}| = \text{Max}\,|A\mathbf{x} - \mathbf{b}|$$

will be minimized. If we put

$$w = \text{Max}\,|e_i|$$

a set of n non-negative constants α may be found such that

$$\alpha A + w > \quad \mathbf{b}$$

and

$$-\alpha A + w > -\mathbf{b}$$

In practice, the problem is treated through the dual problem which is to find non-negative values $\mathbf{x}^+$ and $\mathbf{x}^-$ which maximize

$$\mathbf{b}^T(\mathbf{x}^+ - \mathbf{x}^-)$$

subject to the constraints

$$A(\mathbf{x}^+ - \mathbf{x}^-) < 0$$

and

$$\sum_i (x_i^+ + x_i^-) < 1$$

5. Discussion

5.1. Influence of the Cell Cutting

5.1.1. Size of the Cells. A problem of size arises when one wants to determine the structure producing an anomaly of the gravity field. Two limitations are provided directly by the data. First there is the extent of the anomaly which offers an upper bound and second there is the sample interval between data points which, by way of the Nyquist criterion, imposes the lower bound. This is quite trivial. The reason is, however, not clear from the theorical view point: the size of each cell must be related not only to the sample interval, but also to the ratio between depth and width of the cells. This has been clearly shown by Bott and Hutton (1970) who favour a ratio of depth/width of 1.5 or 2.0.

Bott (1973) calculated the condition number of the matrix kernel for different cases and showed that it passes through a maximum when the field point position is exactly above the centre of the cell. This may cause some problems, and it has been corrected in the sense that a slight shift has been included during the sampling.

5.1.2. Depth. Some variation in the accuracy of the method is related to the estimate of the depth of the real structure. Some tests have been made with a synthetic case in order to show this problem. The anomaly produced by a rectangular structure has been calculated and the data were used as input to the inversion (Fig. 5). In fact, when the cells are exactly at the same depth as the model, the density contrast is estimated correctly by the method. But when the top of the cells in the inversion is lower than the top of the original model, the method of inverting shows, for all norm criteria, a tendency to oscillate around the real values of the density contrast. On the other hand, when the bottom of the cells is situated above the bottom of the original model, a smoothing effect appears in the density contrasts determined by the various methods. This effect of either smoothing or oscillating is a consequence of the equivalent layer

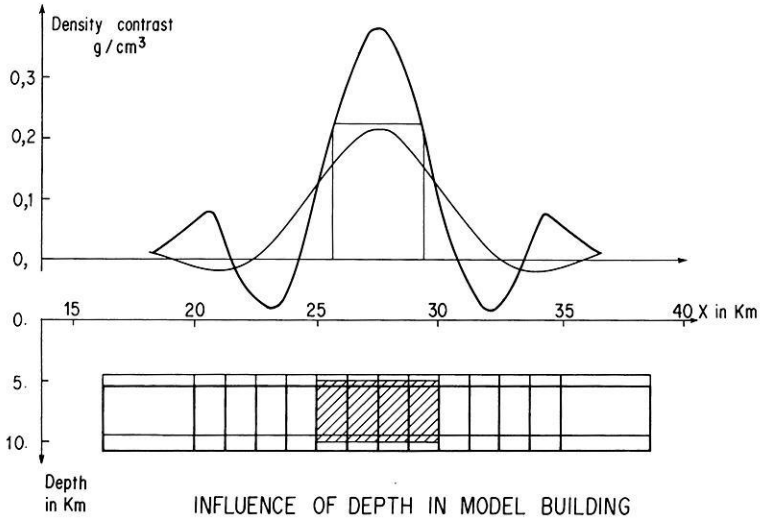


Fig. 5. Influence of depth in model building. Model is hatched. Two layers of cells are shown, one too shallow (thin lines) and one too deep (thick lines). The corresponding computed density contrasts are also shown by thin and thick lines, respectively. Very thin line = true density contrast

theorem. It can be used in its opposite sense in order to correct the estimated depth of the structure. A supplementary hypothesis can be introduced which supposes that the structure is nearly homogeneous with respect to the density contrasts, i.e. that their variations are smooth. This can be tested with other geophysical data available, or with the help of geological information. If upon inverting an anomaly with some arbitrary layer position, oscillations appear in one layer then the model is probably above this layer; if, in contrast, smoothing affects the layer then one has to lower it in order to find the model.

5.1.3. Geometrical Parameters. In a more general way, the above properties of smoothing are still present when an improper shape for the definition of the structure is used. This can be shown by using the triangular cells for approximating a rectangular model (Fig. 6). The calculations give a solution for the density contrast which is quite exact for the central cell; values for cells outside the model are nearly zero, which is correct. The density contrasts calculated for cells overlapping the model are half the theorical values, but the cell volume is doubled; then, by cutting this somewhat arbitrary cell into two pieces one obtains the correct solution.

5.2. Influence of the Norm Criterion

The main aim of this paper is the comparison of different methods of approximation commonly used in order to decide whether the least-squares or the least first power or the minimax solution is the more convenient in geophysical data

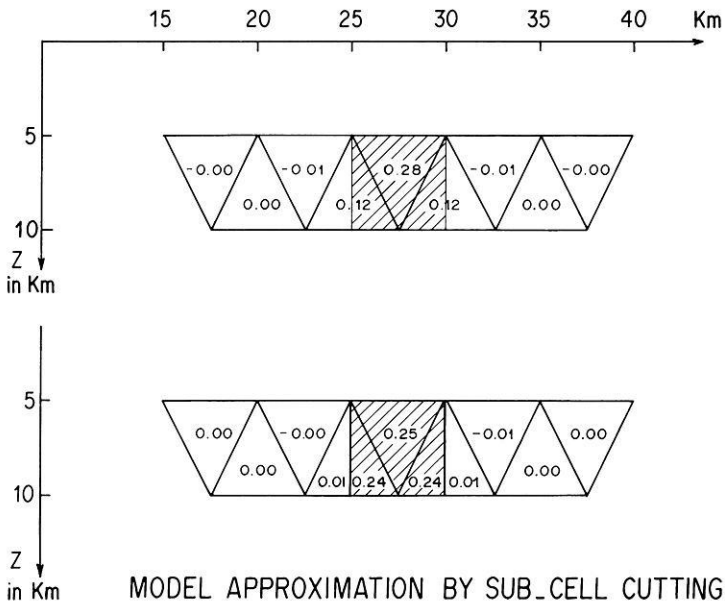


Fig. 6. Model approximation by sub-cell cutting. The model is represented by the hatched square. By cutting two of the adjacent triangles, the true model is more precisely defined

inversion. For this end, a comparison of the different methods has been made using the same test cases, but varying the initial conditions. In fact, no noticeable difference exists when the model is very simple or noise is not included in the data. It seems evident that this very theoretical case could not lead to a successful comparison, although some trouble may arise from the size of the matrix to be inverted. In such cases, it appears that the minimax solution may quickly become unstable or may show a very poor convergence. In cases where the matrix is very large, the author thinks that no comparison can effectively be made between norm criteria, and that the only objects which are compared are the algorithms. Let us take for exemple the usual matrix inversion either by Jordan elimination or by Gauss-Seidel iterations. In the case of a large matrix the first algorithm fails while the second may succeed, but this does not tell anything about the validity of the method for inverting a "small" ill-conditioned matrix.

In order then to compare the methods of approximation, stability has been tested by using noisy data. A synthetic case has been computed, and then random errors with increasing noise level have been added to the synthetic data until each of the three methods fails (Fig. 7). Random errors with a definite noise level have been selected rather than coherent noise. The former can be regarded as a degree of accuracy in the measurements. Several runs give the different density contrasts computed by each algorithm of inversion. No precise level can be determined above which the method fails; it depends on the noise distribution. Anyway, using the same data, methods of inversion can be compared.

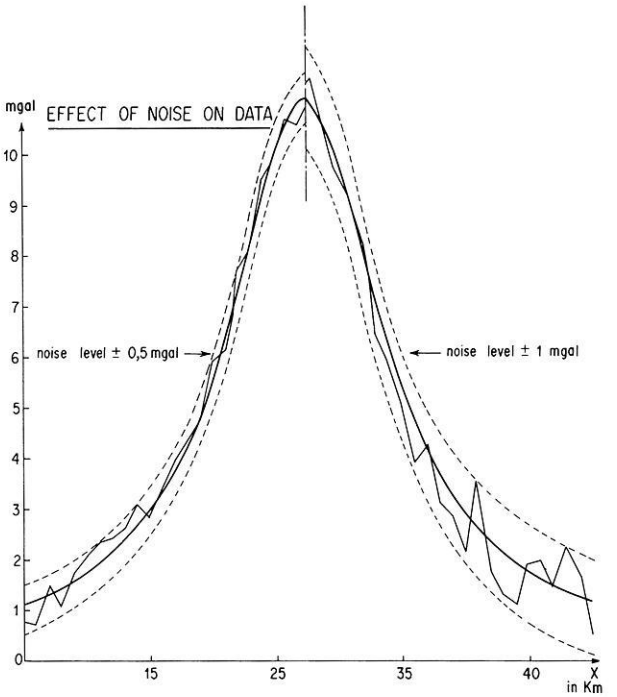


Fig. 7. Effect of noise on data. Two noise levels are represented by the dashed line envelopes. Heavy black line represents the data, thin lines are the noisy data with 0.5 mgal (left) and 1.0 mgal errors (right)

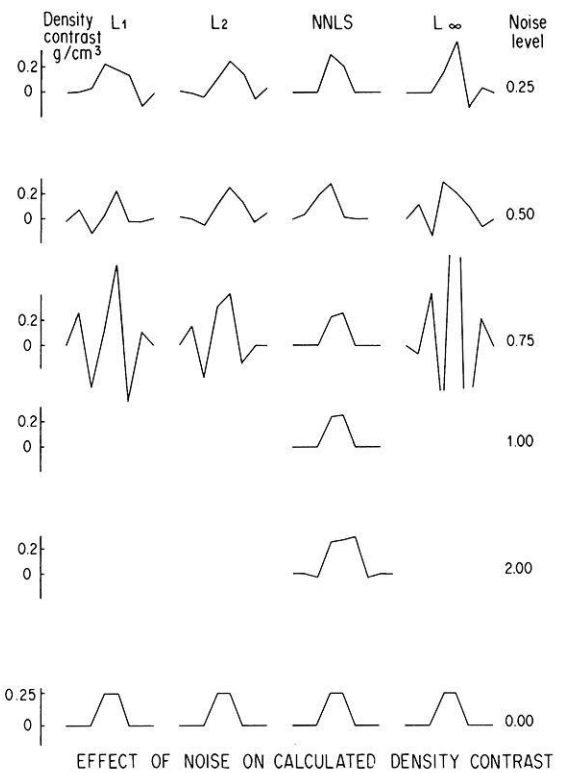


Fig. 8. Effect of noise on calculated density contrasts. Model is defined by eight cells. Source is represented by the two central cells and shows a density contrast of 0.25 g/cm^3, the calculated density contrasts of each of them are represented for the different norm approximation methods (least first power l_1, damped least squares l_2, non-negative least squares NNLS and infinite norm l_∞), for different noise levels in the data

All density contrasts found are plotted on the same diagram (Fig. 8). It has been quite surprising to observe that no major trouble occured when noise level was raised to 0.5 mgal, which corresponds to about 5% error of the maximum amplitude. The Chebyshev approximation is the first to fail at this level, then the least-squares and finally the l_1 method begins to oscillate seriously at 1.0 mgal noise level (maximum 10% of amplitude). The least-squares method has a curious behaviour: it may oscillate at quite low noise level and then may show normal results and once more may oscillate at a higher noise level. This is interpreted as the effect of conditioning of the matrix. For that reason, it is argued that the least-squares method must be seriously looked at before using it in computer programs: no serious troubles are expected from the method itself but in some particular cases it may become unstable while other runs with very similar data show almost perfect results. However, the modification of the classical least-squares method using the Levenberg-Marquardt algorithm seems to be more efficient that the cut-off process of Wiggins (1972).

Another modification of the basic algorithm is possible by the introduction of supplementary constraints on the linear system. This can be done either through inequality conditions or by a non-negativity condition upon the solution. This supplementary condition is in fact of great interest for the gravity inversion problem since it allows the density contrasts to be restricted to values which can be estimated form other data, e.g., seismic velocities or other available geophysical data. In practice, the results are strongly stabilized as shown in the diagram in which all results are compared (Fig. 8). Non-negativity of the results has been used, together with least-squares approximation. With this improvement, noise level may be raised as high as 2.0 mgal (20% of maximum amplitude). It is thought that this method of solving the inverse problem should be developed, since it is of great interest and great stability; but theoretical work on numerical analysis and computer application is still needed. Work would have to be done by using absolute value minimization with introduction of supplementary constraints upon the solution of the inequality type.

A point important to the method, since it has been the cause of much trouble, is the size of the matrix which has to be inverted. From the above definitions, the coefficient matrix depends on m, the number of data points for the columns, and on n, the number of cells chosen to represent the rows. It seems evident that the number of data points is directly related to the frequency content of the anomaly and indirectly related to the shape of the structure. For that reason a large number of data points is needed to represent the spectrum of the source with sufficient accuracy; this leads to quite a large number of columns. If the number of cells remains constant, it leads to more overdetermination, i.e. to more constraints. In practice, it appears that the system may be very unstable in the inversion if overdetermined too much. On the other hand, if the number of rows is increased such that the matrix becomes nearly square, then the size of the matrix may cause the inversion to fail. This problem appears to be the most serious one found in the method. One has always to make a judgement as to how many data must be chosen for the desired precision of the structure and how many cells can be chosen to secure the inversion stability.

Conclusions

The major emphasis of this work has been laid on the way of computing the pseudo-inverse of the coefficient matrix. A general conclusion is that the method of inversion is far more important than the way the matrix has been built. Hence, the results will be very sensitive to which optimization criterion has been chosen. Some care must be taken in the calculation of the coefficient matrix. This is directly related to the problem of conditioning of the matrix. Some precautions are to be taken with respect to the size of the problem taken into account. In fact, this kind of problem is general to all programs of interpretation, it is really a matter of selecting the degree of precision of the solution with respect to the accuracy of the data.

Several conclusions can be drawn from the comparison of the different algorithms of approximation. As was anticipated, the infinite norm approximation is not the best way to approach the problem. It is very sensitive to errors in the data and seems to be quite unstable if a priori information about the supposed structure is missing. A more interesting way to solve the inverse problem seems to be through the least first-power algorithm. It offers the advantage over the usual least-squares approximation of being less time consuming for better precision in the results. This point comes from the stability of the method with respect to errors in the data. In fact, this can be related to the way of doing the decomposition in the simplex method of all vectors in two parts, each one being positive.

An interesting conclusion is related to the introduction of constraints in the least-squares approximation. Imposing non-negativity on the solution is in fact the only way to stabilize the solution. This is directly related to the supplementary condition of convexity of the solution. The set of all solutions is now reduced to the semi-infinite set of solutions positive, and this suffices to greatly stabilize the solution. A suggestion is then made to build some new kind of algorithm in order to use the condition of convexity of the solution, by introducing constraints upon the range of values for the solution. This could be tested easily with the least-squares approximation and then could be introduced into the first-power algorithm.

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