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Damped and Constrained Least Squares Method With Application to Gravity Interpretation

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Abstract. Many geophysical problems are solved through linear system inversion techniques. Optimization routines are the usual schemes and among them the least-squares method is the most common. Some refinements as matrix decomposition, elimination of insignificant eigenvalues are considered and tapering of small eigenvalues is proposed. The introduction of an upper and a lower limit for the solution vector is presented. This reduces the usual instability encountered when using classical least squares techniques.

An application to gravity profile inversion shows how this method can be used as an intermediate between the direct problem (model construction) and the inverse problem (search for ideal bodies).

Key words: Constrained least squares – Inverse problems – Gravity.

I. Introduction

Provided an appropriate choice of the parameters, a lot of geophysical problems may be reduced to a linear combination of relationships between the measurements b of physical quantities and a set of unknown parameters x. The problem is to solve the linear system

$$Ax = b \tag{1}$$

in order to find the solution vector x representing the unknown parameters x_j. Since the number m of observation points b_i does not need to be equal to the number n of the different physical parameters to be determinated, the system $Ax = b$ must be solved using an approximation theory. A good solution is

$$b' = b + e\, Ax \tag{2}$$

with e being the residuals between computed and observed values. The problem is then to reduce the values of the residuals, that is to say to minimize the

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quantity $\|Ax-b\|$. Several criteria are available, dealing mainly with the power used to calculate the norm. Some of them have been examined in a previous paper (Vigneresse, 1977). Here only least-squares approximations are presented.

2. Theory

2.1. Classical Least Squares

Resolution of the system can be obtained by the usual Gauss method. Normal equations can be written

$$A^T A x = A^T b. \tag{3}$$

The solution is given by

$$x = (A^T A)^{-1} A^T b. \tag{4}$$

Troubles arise from the computation of the inverse of $A^T A$. Instabilities occur when the A matrix is badly conditioned, since the condition number of $A^T A$ is the square of the condition number of A. This may cause serious problems during the inversion (Anderssen, 1969).

2.2. Matrix Decomposition and Damped Least Squares

Lanczos (1961) proposed an improvement by using an eigenvalues-eigenvectors decomposition of the matrix

$$A = USV^T. \tag{5}$$

Solution is now obtained by

$$x = VS^{-1} U^T b. \tag{6}$$

U and V are orthogonal matrices whose columns are the eigenvectors associated with the columns and rows of A respectively. S is in this case a diagonal matrix, the elements of which are the eigenvalues of the full rank matrix. If degeneracy occurs some eigenvalues are equal to zero. In the numerical application, the existence of small eigenvalues comes from irrelevant and unimportant parameters.

It can be desirable to keep these low eigenvalues during the inversion for instance when the effects of several parameters are very similar and are hardly distinguishable from the data. (Levenberg, 1944; Marquardt, 1963, 1970). The method is also known as ridge regression (Hoerl and Kennard, 1970).

The normal Eq. (3) are modified to

$$(A^T A + \Theta I) x = A^T b \tag{7}$$

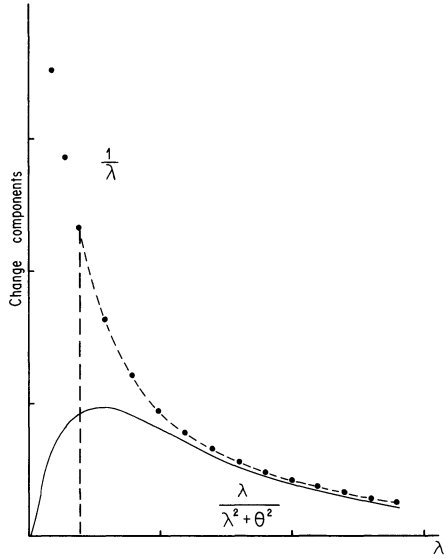

Fig. 1. Eigenvalue spectrum obtained by using classical least squares inversion ($1/\lambda$, dots), threshold value (broken line) and damped least squares as described in present paper ($\lambda/\lambda^2 + \Theta^2$), solid line)

where Θ is a diagonal matrix with positive elements. When using the same type of matrix decomposition as previously (5) the normal equations are written

$$(VS^2U^T + \Theta I)x = VSU^Tb \tag{8}$$

and a solution is

$$x = V|(S^2 + \Theta^2 I)^{-1}S|U^Tb. \tag{9}$$

The effect has been the introduction of a perturbation factor Θ^2 which tapers the spectrum of the eingenvalues (Fig. 1). A scheme of calculations is provided in Table 1.

The choice of a convenient value for Θ is essential. A good estimate is given by weighting the residuals by one over the variances of the observations (Crosson, 1976). This leads to a normally distributed random variable with unit variance. Aki and Lee (1976) use a weight inversely proportional to the variance, namely the ratio of the variance of the data over the variance of the estimated solution. The same choice had been proposed by Franklin (1970) in the method of the stochastic inverse.

2.3. Constrained Least Squares Approximation

In spite of these improvements, the least-squares problem does not have unique solution in the overdetermined case, and the solution may be optimum only in the mathematical sense, i.e.: it can be physically out of range even if the criterion of minimizing the sum of squares of the residuals is fully satisfied. From a geophysical point of view, it would be better to choose a solution within an average range of physically meaningful values.

Table 1. Scheme of resolution of overdetermined system through classical and improved least squares minimization

System $Ax = b$

	CLASSICAL LEAST SQUARES	LEVENBERG _ MARQUARDT DECOMPOSITION
Minimization of	$(Ax-b)^T\ (Ax-b)$	$(Ax-b)^T\ (Ax-b)+\theta^2\ x^T x$
Normal équations	$A^T A\ x = A^T b$	$(A^T A+\theta^2 I)\ x = A^T b$
Solution	$x = (A^T A)^{-1} A^T b$	$x = (A^T A+\theta^2 I)^{-1} A^T b$
MATRIX DECOMPOSITION		
	$A = U S V^T$	$A = U S V^T$
Normal équations	$V S^2 U^T x = V S U^T b$	$(V S^2 U^T+\theta^2 I)x = V S U^T b$
Solutions	$x = V S^{-1} U^T . b$	$x = V\{(S^2+\theta^2 I)^{-1} S\} U^T b$
	$S^{-1} = \begin{vmatrix} 1/\lambda_1 & & 0 \\ & 1/\lambda_2 & \\ 0 & & \ddots\ 1/\lambda_n \end{vmatrix}$	$(S^2+\theta^2 I)^{-1} S = \begin{vmatrix} \frac{\lambda_1}{\lambda_1^2+\theta^2} & & \\ & \frac{\lambda_2}{\lambda_2^2+\theta^2} & \\ & & \ddots\ \frac{\lambda_n}{\lambda_n^2+\theta^2} \end{vmatrix}$

(a) *Theory.* The introduction of such limits for the solutions can be formulated as the following Constrained Least-Squares problem (CLS problem):

$$\text{Minimize } \|Ax-b\| \text{ subject to } Cx>d \tag{10}$$

with the $m \times n$ matrix A, equivalent to the above notation, and the $p \times n$ matrix C of the relations between the constraints vector d and the solution vector x.

Two particular cases of this problem are evident:

Problem LDP (Least Distance Programming):
Minimize $\|x\|$ subject to $Cx>d$ (11)

Problems NNLS (Non Negative Least Squares)
Minimize $\|Ax-b\|$ subject to $x>0$. (12)

An algorithm for NNLS problem has been dealt with, and solved, in linear and non-linear programming. Basic theorems are found in the original paper by Kuhn and Tucker (1951) and in books dealing with optimization (Laurent, 1972; Fiacco and McCormick, 1968). Applications and practical use have been developed by Lawson and Hanson (1974), and by Gill and Murray (1974).

Kuhn and Tucker (1951) solved the CLS problem by introducing slack or surplus variables (r) in order to reduce the inequalities in $Cx>d$ to the equalities $Cx-r=d$ with the condition $x, r>0$. The problem of minimizing $\|Ax-b\|$ can be treated using the objective function $\phi=\frac{1}{2}\|Ax-b\|^2$. Saddle-point theory applied to ϕ then provides a set of necessary conditions. Kuhn and Tucker (1951) derived from it what they referred to as "constraint qualification", which places very important restrictive conditions on the nature of the set of feasible solutions in the vicinity of the computed solution x^+. It requires that the negative gradient vector of ϕ at x^+ must be expressed as a non-negative linear combination of outward pointing normals to the constraint hyperplanes on which x^+ lies. That is to say, that it lies in the convex cone based at the point x^+ and generated by the outward pointing normals. More recent works on functional analysis have developed this point and stress the optimization problem through the intersection of cones of displacement (Laurent, 1972).

For the CLS problem, a solution is then characterized by the following conditions (Lawson and Hanson, 1974): An n vector x^+ is a solution of the CLS problem if and only if there exists an m vector y and a partitioning of the integers 1 to m into subsets E (equality) and S (slack) such that

$$\begin{aligned} &C^T y = A^T(Ax-b) \\ &r_i=0; \quad y_i>0 \quad i\varepsilon E \\ &r_i>0; \quad y_i=0 \quad i\varepsilon S \quad \text{where } r=Cx-d. \end{aligned} \tag{13}$$

The quantity $-|A^T(Ax-b)|$ is then the negative gradient of the objective function $\phi=\|Ax-b\|^2$ and the lines of $(-C^T)$ represent outward pointing normals to the constraint hyperplanes.

If the NNLS problem may be solved, the point is now to reduce the CLS problem to the NNLS problem. This is done in two steps: reduction of the CLS problem to the LPD problem, and then change of the LDP problem to the NNLS problem.

(b) *Practice.* The reduction is carried out with the help of matrix decompositions as described in the first part of the present paper. An advantage of this procedure is a single singular-values analysis in the first step of the computation.

The first step is done through a change of basis for the vector x. The matrix decomposition which leads to $A=USV^T$ Eq. (5) can be written

$$|A| = |U_1\, U_2| \begin{vmatrix} S & 0 \\ 0 & 0 \end{vmatrix} \begin{vmatrix} V_1^T \\ V_2^T \end{vmatrix}. \tag{14}$$

Then by a change of variables $x=V_1 y$, the problem of minimizing the quantity $\|Ax-b\|$ reduces to:

$$\begin{aligned} &\text{minimize } \phi=\|b-Ax\|^2=\|-Sy+b_1\|+\|b_2\| \\ &\text{with} \qquad b_1=U_1^T b \\ &\qquad\qquad\;\; b_2=U_2^T b \end{aligned} \tag{15}$$

A further change of variables $z=Sy-b_1$ reduces the function to

$$\phi=\|z\|^2+\|b_2\|^2. \tag{16}$$

The problem is now reduced to the LDP problem, except for the additive constant $\|b_2\|^2$:

$$\begin{aligned} &\text{Minimize } \|z\| \text{ subject to } \hat{C}z>\hat{d} \\ &\text{with} \qquad\qquad \hat{C}=CV_1S^{-1} \\ &\qquad\qquad\qquad\;\; \hat{d}=d-CV_1S^{-1}b_1. \end{aligned} \tag{19}$$

The second step is the transformation from the LDP to the NNLS problem. This can be done through the following change: compute a vector u solving the NNLS conditions:

$$\text{Minimize } \|Eu-f\| \text{ subject to } u>o \quad (18)$$

with $E=\begin{vmatrix}\hat{C}^T \\ \hat{d}^T\end{vmatrix}$ and f an $n+1$ vector with all elements equal to zero except $(n+1)$ th.

The gradient vector of the objective function $\frac{1}{2}\|z\|^2$ in the LDP is simply z. The Kuhn-Tucker conditions require z to be expressible as a nonlinear combination of the row of $\hat{C}^T$. Then z is expressed as

$$z=\hat{C}^T u\|r\|^{-2} \quad \text{with} \quad \|r\|^2=r^T r=r^T\|Eu-f\|. \quad (19)$$

3. Application to Gravity Data

Gravity profile interpretation may be aided through linear system inversion techniques. Two-dimensional density distributions can be selected to represent geological structures. The gravitational attraction due to simple sources represented by polygons is easily calculated by the now classical formula of Talwani et al. (1959). Since the formula is linear with respect to density, a linear system of equations can be constructed yielding a theoretical gravity value at any point. Provided that observed gravity values are available at these points, density contrasts can be adjusted in order to minimize the residuals between observed and computed values of the field.

The assumed structure which underlies the gravity anomaly is divided into several cells by an automatic partitioning or by a more elaborate method which can incorporate results from previous geophysical surveys. Each cells is then represented by a regular polygon.

The gravitational attraction of a k-sided polygon is given by

$$g=2G\rho\sum_{l=1}^{k} Y_l. \quad (20)$$

Where G is the universal gravitational constant and ρ the density. Y_l is the kernel function for one side and is a function of x_l, z_l, corners of the polygon.

The problem reduces to a linear system like Eq. (1) with the solution vector $b=g_i$ the gravity measurements, the unknown vector $x=\rho_j$ the density contrast, and the matrix $A=aij$, represents the gravitational attraction of the j^{th} prism at the i^{th} point of observation. Details of constructing this system may be found in a previous paper (Vigneresse, 1977).

4. Discussion

The inverse problem in gravity interpetation has already been examined by these techniques. To date, several papers have been published, each using different criteria for the optimization of the residuals.

In a first stage, most of the authors have assumed density contrasts and adjusted vertical coordinates of the bodies by means of either iterative processes (Tanner, 1967; Qureshi and Mula, 1971) or least-squares methods (Corbato, 1965). Later, methods with better convergence have been developed through least-squares techniques and generalized inversion (Braile et al., 1974; Philips, 1974; Jupp and Vozoff, 1975). The problem of stability has been partially solved by the Backus and Gilbert (1967, 1968) method (Green, 1975) and by ridge regression (Inmann, 1975). Different criteria for norm minimization have been proposed (Claerbout and Muir, 1973) and compared with each other (Vigneresse, 1977). As far as errors in the data affect the solution, the problem is better solved with the introduction of a damping factor in the least-squares approximation (Crosson, 1976; Aki and Lee, 1976) or using covariance matrix techniques (Jackson, 1976; Burkhard and Jackson, 1976).

From the point of view of the very recent development of the inverse problem (Parker, 1975, 1977; Sabatier, 1977a and b), the method described above may certainly be considered as "old fashionned". The fact is that Parker's philosophy of determining all solutions acceptable for the problem is very reasonable. Unfortunately, this is very time consuming (Sabatier, 1977a). Another point is the basic assumption of a homogenous structure underlying all these methods. Any geologist will have serious criticisms about this. These are the main reasons why the present method has been developed.

When inverting real data, both oscillations and smoothing effects occur but they may be used in order to approach a "better" solution. A solution remains to be found in which the density contrasts are limited within a physically acceptable range, taking into account the other available data for the structure. In that sense the method can be viewed as a compromise between an arbitrary search through model calculations (direct method) and a mathematical inverse problem (automatic adjustements of depth parameters).

The method has been tested with several synthetic models. In all cases the inversion was done in a very short time and gave the previously assumed density contrasts.

In order to simplify the procedure, the same test has been done for several runs in the computer with different initial parameters. An ideal structure had been computed by the usual Talwani et al. (1959) method. It seemed interesting to take the same test model as used by Braile et al. (1974) in order to compare the accuracy (Fig. 2).

Furthermore a test has been made by introducing random noise in the synthetic data. The noise level was progressively raised in order to observe the failing of the method. Up to a noise level of approximatively 20%, the results are within an acceptable range. In fact this follows from the implicit supplementary constraints which result from the location of the geometrical parameters of the model. If a set of cells has exactly the shape of the test model then inversion can be done up to high noise levels. When the division into cells does not approximate the model exactly, however, some differences are found during the least-squares inversion. With respect to the depth, a lower bottom for the structure causes the density contrasts to oscillate while they are smoothed when the top to the structure is higher than that of the model. Such troubles are

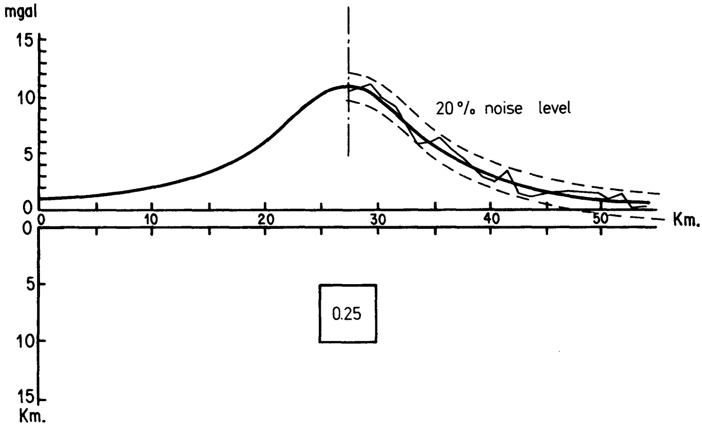

Fig. 2. Test model in the present paper. On the right hand side noise has been added with a noise level of 20%

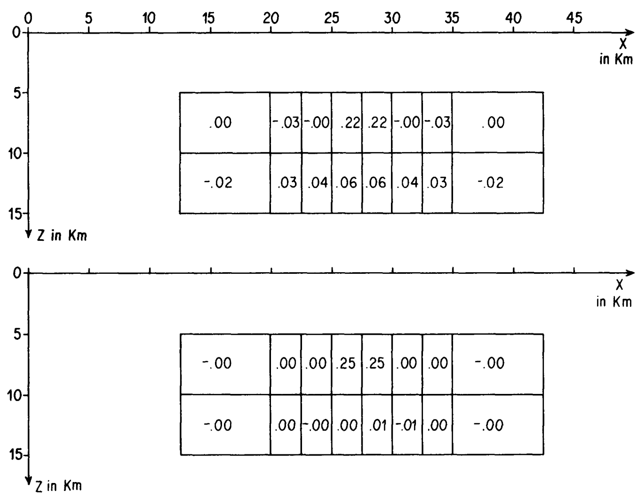

Fig. 3. Test model anomaly inversion. (*a*) damped least squares method; (*b*) constrained least squares method. Upper bound was 1.00 g/cm^3 and lower bound -1.00 g/cm^3

nearly always found during least-squares inversion, but the introduction of constraints reduces the amplitude of the variations. Smoothed values occur only when the structure is higher than the source, which is probably due to the equivalent-layer theorem. Lateral displacement of the cells may affect the result, though in fact only the edges of the structure are affected. If a cell comprises part of the model as well as the host rock, a density contrast which combines their respective densities will be assigned by the procedure. If one cell overlaps the model, then it will be given a density contrast result of a combination of both density contrasts of the model and surrounding structures. The introduction of constraints upon the solution vector severely reduces the instability during the inversion. An exemple is presented in Fig. 3. The test model anomaly is inverted using both techniques of damped least squares and constrained least squares. The cell structure chosen fits the cell shape, but its lateral extension is less than the length of the profile. This results in a long wavelength instability which manifests itself in an ill conditioning of the coefficient matrix (Vigneresse, 1977). In the damped case, the computer tries to fill the lower cells in order to deal with the long wavelengths. The result is shown in Fig. 3a. The constrained inversion was done using a density contrast of $+1$ and $-1\,g/cm^3$ as upper and lower bounds, respectively. The instability is reduced as one can see in Fig. 3b. The introduction of constraints into the solution results in the construction of a convex hull into which all feasible solutions for the problem fall. In that sense the problem can be viewed as a convex rather than a linear problem (Sabatier, 1977a).

5. Applications

The present method has been developed for a specific geological problem. For a long time, geologists have been interested in the determination of the shape of the roots (bottom) of batholiths.

Gravity data can assist in this problem by calculating the shape of a batholith. This has been done by several authors using different methods. The main point is still unsolved because of a dogmatic assignment of the density contrast; it is generally assumed that the structure is homogenous and does not show variations in its physical parameters. Though it is quite easy to estimate the density contrasts existing at the outcrops, only assumptions are available for depths as great as some ten kilometers as inferred by several authors. Therefore, the determination of the structure, from a continuity in their density contrasts could be a less biased approach to the problem of plutonic roots.

Data are taken from the gravimetric anomaly map of Brittany, western France. Plutons are well known in this area; they consist of leucogranitic rocks dated from 310 m.y. (Cogné, 1974). They are easily recognisable on the Bouguer anomaly map as they are delineated by negative anomalies of some -25 mgal. Density contrast measurements have been carried out on their material (Weber, 1972); an average value for the granite is $2.61\,g/cm^3$ while the palaeozoic formations into which they intruded have a mean density value of $2.69\,g/cm^3$; this results in a gravity contrast of $-0.08\,g/cm^3$ between the granite and surrounding rocks. A profile has been constructed across the Guehenno massif (Fig. 4). Constraints have been placed upon the solution vector. Density constrast is allowed to vary within the range $-0.12\,g/cm^3$ and $+0.05\,g/cm^3$. Inversion has been carried out through the above methods. Results have been compared with other automatic inversion processes (Tanner, 1967; Qureshi and Mula, 1971) (Fig. 5).

A few comments can be made on the results; since the decomposition into cells has been very crude. The decomposition presented shows a similar shape to that of the other methods. It results from several trials with more general

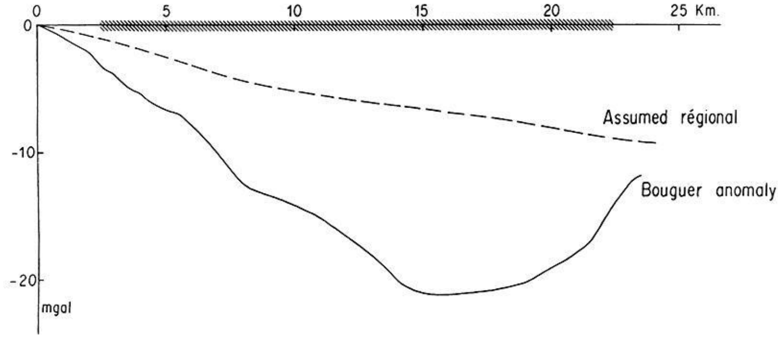

Fig. 4. Bouguer anomaly profile over a granitic pluton. Outcrops are indicated with hatches and measured surface density shown

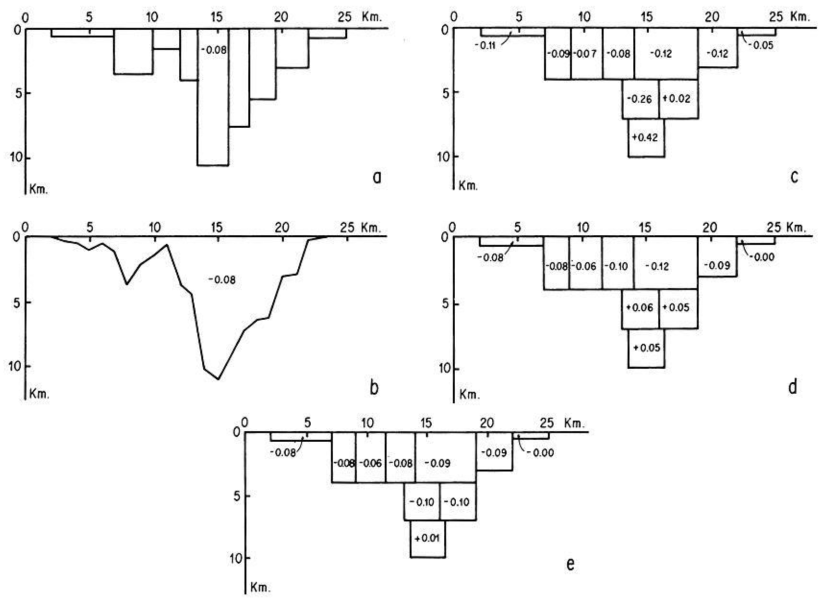

Fig. 5. Diagram showing the results of different methods of inverting gravity data. (*a*) Tanner's (1967) method; (*b*) Qureshi and Mula's (1971) method; (*c*) the classical least squares inversion; (*d*) a damped least squares inversion using Levenberg Marquardt's algorithm; (*e*) results from the constrained least squares optimization. Constraints have been choosen as -0.12 g/cm^3 and $+0.05$ g/cm

divisions. After two runs, convergence of the results leads to this structure. A first comment is the similarity of the results between all the three methods concerning the shape of the batholith. No problem is encountered here. However a significant difference occurs with respect to the depth of structure. Classical inversion methods for a structure having constant density throughout the body (i.e., homogeneity in its density contrast) indicate a greater depth for the root than the one computed through our inverse method. But the density contrasts calculated by our method change with depth, thus, the batholith may be homogeneous from the point of view of the petrologist, but not for geophysicist. This may result from a density contrast between the body and the host rock which changes gradually from the surface (at the outcrop) to deeper levels in the upper crust.

Conclusions

A method has been developed which solves the gravimetric inverse problem by a linear least-squares approximation. Refinements to the classical method of matrix decomposition have been incorporated. The principal feature is the tapering of the eigenvalue spectrum, avoiding the effect of redundancy in the data. A supplementary and powerful condition is used assigning the convexity to the solution. Assuming that other available data allows a restricted range for the density contrasts, the solution is constrained to lie within that range. The introduction of such constraints during the computation severely stabilizes the method of matrix inversion and allows reasonable solution with limited time consumption. Tests upon synthetic models are significant even when noise is introduced into the data. When used upon real data the method shows good performances compared to other iterative methods of gravity interpretation.

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