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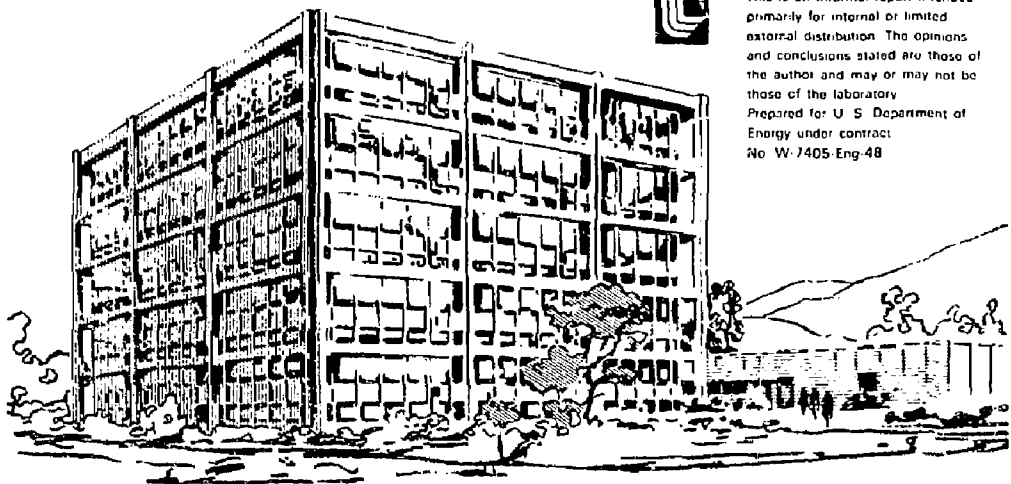
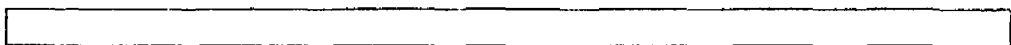
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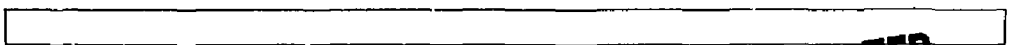
GRAVITY INVERSION CODE

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February 1, 1979



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GRAVITY INVERSION CODE

ABSTRACT

The gravity inversion code applies stabilized linear inverse theory to determine the topography of a subsurface density anomaly from Bouguer gravity data. The gravity inversion program consists of four source codes: SEARCH, TREND, INVERT, and AVERAGE. TREND and INVERT are used iteratively to converge on a solution. SEARCH forms the input gravity data files for Nevada Test Site data. AVERAGE performs a covariance analysis on the solution. This document describes the necessary input files and the proper operation of the code.

INTRODUCTION

The gravity inversion code applies stabilized linear inverse theory to determine the topography of a subsurface density anomaly from Bouguer gravity observations. The program assumes that the topography takes the form of a step function in two dimensions, and it compares model predictions directly with the Bouguer gravity data (no smoothing or interpolation is necessary). The program then determines the resolving kernels for the gravity data (characteristic of the non-uniqueness in the gravity data) and the error in the model estimates.

The gravity inversion program consists of four source codes: SEARCH, TREND, INVERT, and AVERAGE. SEARCH forms the input gravity data sets from the Nevada Test Site (NTS) gravity data file HEALEYNTS. TREND forms the partial derivative matrix for the linear inversion code INVERT. INVERT formulates a solution using stabilized linear inverse theory. AVERAGE performs a covariance analysis on the solution. The four source codes and HEALEYNTS are stored on the Lawrence Livermore Laboratory's Octopus system. The file directory name is 120750:GRAV.

Although specifically designed for NTS gravity data, the inversion program will invert Bouguer gravity data from any basin. The model for

the basin consists of right rectangular prisms having a common top elevation and variable depths. Density contrasts are specified for each prism.

TREND and INVERT are used iteratively to converge on a solution. TREND takes all the input data and creates a disk file (OUI) that is used as input to INVERT. This division of the source code permits an analyst to experiment with different constraints on the solution or with different tradeoff points in the resolution vs variance curves without recalculating the partial derivative matrix.

SOLVING THE PROBLEM

Burkhard and Jackson¹ have documented the method employed in TREND and INVERT to form the partial derivative matrix and to formulate the solution, respectively. Inversion of gravity data for depth is a non-linear problem; INVERT solves the linear approximation to the non-linear problem. The discrete linear inverse theory used in INVERT handles the overdetermined problem (i.e., there are more data than unknowns) instead of the underdetermined case that is documented in Ref. 1. To use the TREND and INVERT codes, the user must have a working knowledge of linear inverse theory.

These codes assume that the gravity anomaly is accurate only to within an additive constant (i.e., a constant value can be added to all the gravity data without changing the shape of the anomaly). INVERT automatically solves for an additive gravity constant, and in doing this, finds a basement topography that would generate an anomaly matching the shape of the actual gravity anomaly, although not necessarily matching the values of the actual data. INVERT finds the "basement" topography by solving for perturbations to an initial model. Thus, the final solution is a function of the initial model.

LINEAR INVERSION THEORY

INVERT uses a stabilized linear inversion scheme. Stabilization is achieved by introducing the initial model as data weighted by the

stabilization parameter. First, the program calculates a solution for a given value of the stabilization parameter; then it calculates constrained solutions as linear perturbations of the initial solution. The Cholesky square-root method is used to find the inverses of the symmetric matrices. The inversion scheme minimizes the quadratic form s^2 subject to some linear constraint equations.

$$s^2 = \epsilon^T \epsilon + \lambda_o^2 x^T x + K^T (Bx - DN) \quad (1)$$

where

- $\epsilon = y - Ax$
- $y =$ gravity data
- $\lambda_o^2 =$ stabilization parameter
- $x =$ depth of prisms
- $A =$ partial-derivative matrix
- $Bx - DN =$ linear constraint equations
- $K =$ Lagrange multipliers

When we minimize s^2 and solve for x , we get:

$$x = \begin{bmatrix} H_a & \bullet & H_b \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix} \begin{bmatrix} y \\ \bullet \\ DN \end{bmatrix} \quad (2)$$

where $H_a = \begin{bmatrix} I_m & -H_b B \end{bmatrix} H$

$$H_b = M^{-1} B^T K^{-1}$$

where $H = M^{-1} A^T$

$$K = BM^{-1} B^T$$

$$M = A^T A + \lambda_o^2 I_m$$

This method of solution first obtains H (assume $B \equiv 0$). From that, we form H_a and H_b for each set of constraints. The resolution, covariance, and total error are obtained as follows:

- Resolution— $R^* = R + H_b B \left[I_m - R \right]$

where $R = HA$

- Covariance— $C^* = \left[I_m - H_b B \right] C \left[I_m - H_b B \right]^T$

where $C = HH^T$

- Total error— $C_T^* = (R^* - I_m)(R^* - I_m)^T + C^*$

The following rms quantities appear as output from INVERT: EBAR, XBAR, RBAR, SDBAR, and SD TOTAL BAR. EBAR is the average fit of the solution to the real data.

$$EBAR = \bar{\epsilon} = \sqrt{\frac{1}{n} (\epsilon^T \epsilon)}$$

XBAR is the average size of the perturbation x to the initial model.

$$XBAR = \bar{x} = \sqrt{\frac{1}{m} (x^T x)}$$

RBAR is an estimate of the average resolving ability of the data.

$$RBAR = \bar{r} = \sqrt{\frac{1}{m} \|R^* - I_m\|^2}$$

where $\| \cdot \|^2$ means the sum of the squares of elements.

SDBAR is the average error in the parameters.

$$SDBAR = \bar{\sigma} = \sqrt{\frac{1}{m} \|H_a\|^2}$$

SD TOTAL BAR is the average total error (i.e., sum of resolving and propagated data error) in the solution.

$$SD \text{ TOTAL BAR} = \bar{\sigma}_T = \sqrt{\frac{1}{n} |C^*|}$$

where $| |$ is the sum of the diagonal terms (spur of matrix).

The correlation matrix is defined by:

$$\rho_{ij} = \frac{C_{Tij}^*}{\sqrt{C_{Tii}^* C_{Tjj}^*}}$$

This matrix reflects the correlations between the parameters in the solution. The estimates of the resolving power for each model parameter and the estimates of the propagated data error are given by:

$$\tau_k = \sqrt{\left[(R^* - I_m)(R^* - I_m)^T \right]_{kk}}$$

where $k = 1, m$ and there is no sum on k .

$$\sigma_k = \sqrt{C_{kk}^*}$$

where $k = 1, m$ and there is no sum on k .

The quoted \pm value on the solution in OUTBIN are:

$$\sigma_{T_k} = \sqrt{C_{T_{kk}}^*}$$

where $k = 1, m$ and there is no sum on k .

Most-squares solutions are such that the sum of the error is equal to some maximum value, Q_0 (see Ref. 2). In this program, the maximum value

Q_0 is set to $(N + \text{ALPHA} * M)$. One perturbs in the direction given by $x^T b$ (where b is the most-squares vector referenced in the input). The solutions are:

$$x_{ms} = x_{slb} + \mu(H_b B - I_m)M^{-1}b$$

where $\mu = \pm \sqrt{\frac{Q_0 - s^2}{b^T L M L b}}$

$$L = (H_b B - I_m)M^{-1}$$

and define $\mu = 0$ if $\|Lb\| \leq 0$.

The value x_{slb} is the solution of Eq. (2). Note that x_{ms} gives two extreme boundary conditions.

PROGRAM REQUIREMENTS AND OPERATION

Communication with the codes requires several disk files, which are described in detail in the next section. The various parameters contained in the disk files should be selected carefully to preclude problems.

The region is modeled with right rectangular prisms whose horizontal dimensions are established by the input parameters in file IN3. XMOD requires an initial model of the "basement" topography. If the topography is unknown, the program will accept a uniform depth estimate. The density contrast of each prism must be specified in IN4. The gravity of each right rectangular prism is calculated with the Nagy formula.³

In IN3, WX and WY specify the unit dimensions of the grid spacing in kilometres in the X and Y directions, respectively. The integer arrays IWY and IWY specify the separation of the grid lines in terms of

the unit dimensions WX and WY, respectively (see Fig. 1). The grid is automatically centered around the point (COORDX, COORDY). WX, WY, IWX, and IWY should be carefully selected to accomplish several tasks:

- Prisms should be small enough to represent area of greatest interest.
- Grid should be large enough to enclose sufficient area to calculate gravity accurately.
- Number of prisms should be small enough to fit computer core, time, and finite machine-precision restriction.

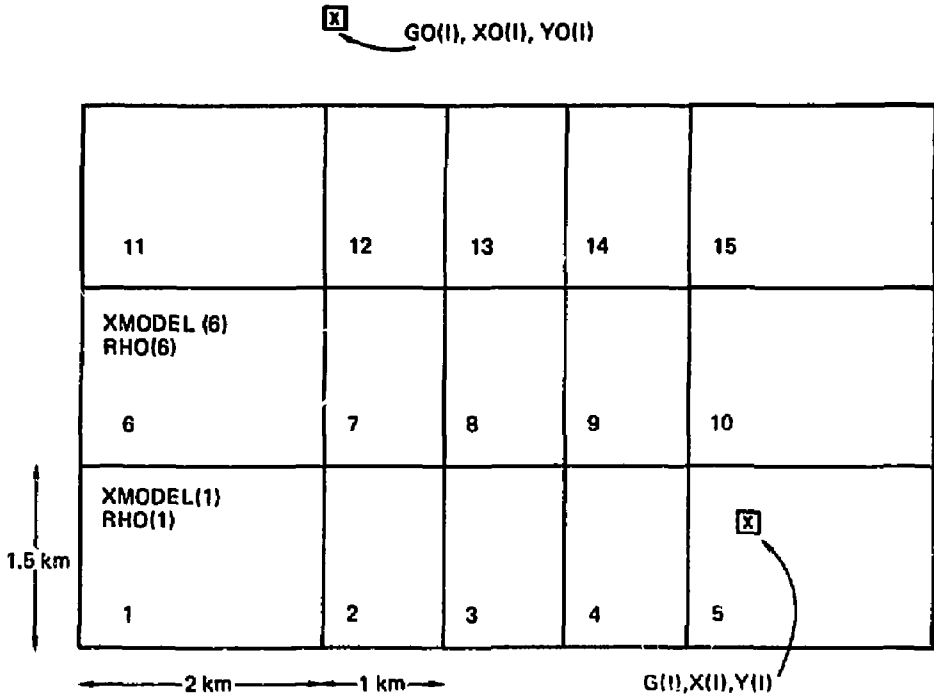
Generally, the grid should extend about five times the depth expected under the gravity values near the edges of the inner data block IN1. Also, resolution is very poor if the average gravity data density is less than one datum per prism.

The covariance-of-error matrix for the Bouguer gravity anomaly and the *a priori* depth-covariance matrix must be specified in IN5 and IN6, respectively. The error in the NTS gravity has been found to range from 0.2-0.5 mgal. Reasonable *a priori* depth uncertainties are 0.3-0.5 km. The *a priori* depth- and gravity-data covariance matrices are used to standardize the unknown parameter and gravity data sets, respectively. Standardization puts the data and parameter spaces into statistically independent and dimensionless forms possessing unit variance.

The codes have no provision for dynamic dimensioning. In order to optimize the computer core requirements, the source codes of TREND and INVERT should be compiled with the appropriate dimensions for the arrays.

The dimensions of the arrays in TREND, contained in source lines 46-52, should be adjusted according to the dimensions given in source lines 36-44 of TREND. NI is the number of data points in IN1 (inner data block); NO is the number of data points in IN2 (outer data block). M is the number of prisms used to model the region. The values of ND and MD in the PARAMETER statement, line 141 of INVERT, should be greater than or equal to N and M contained in line 1 of file OUI.

TREND assumes that the covariance matrix for the data reflects the errors made during correction of the data. TREND further assumes that



$WX = 1 \text{ km}$ $IWX(J) = 2, 1, 1, 1, 2$
 $NX = 5$ $J = 1, 5$

 $WY = 1.5 \text{ km}$ $IWK(K) = 1, 1, 1$
 $NY = 3$ $K = 1, 3$

Fig. 1. Representation of parameter blocks within the program, showing the ordering and sample values used to define the model. All distances (X, Y, X0, Y0) must be positive.

the program user will apply a grid system large enough to represent adequately the region around the data points in IN1. Because gravity anomalies can be uncertain by a constant amount, TREND automatically assigns an additive gravity constant as the last unknown parameter. The starting value of the additive constant is 0.0. TREND also automatically assigns it an a priori variance equal to the variance of the revised data vector.

TREND performs the following calculations:

- Subtracts regional trend from observed gravity data if desired.
- Forms a revised data vector from the difference between the observed data and the calculated data from the starting model XMOD.
- Calculates a partial derivative matrix relating a change in model parameter μ to datum i .
- Standardizes the data vector (i.e., puts data into a statistically independent and dimensionless form possessing unit variance).
- Creates output data file OUI for use as input to INVERT.

INVERT performs the following calculations:

- Formulates a solution with no constraints.
- Formulates a solution with constraints, if desired.
- Formulates resolution and correlation of parameter matrices, if desired.
- Formulates most-squares solutions, if desired.

Operation of the inversion code involves the following steps:

1. Create the necessary data files. This process can be lengthy because several factors must be considered. The rectangular grid of blocks must provide adequate coverage of the area of the data points in IN1. A rule of thumb is that the grid should extend about five times the expected depth from any gravity point. The data in IN2 should cover an area sufficiently large so that the regional trend found will approximate the actual regional trend. Note that the initial model and density contrasts should be listed in the proper order (see Fig. 1).

2. Run TREND once with ITREND = 2 in IN7 if the regional trend data in IN2 has changed, or if several iterations or several different problems using the same regional trend data are foreseen. This will store the regional trend data in disk file TREN and will save calculations in subsequent runs. When running TREND subsequently, set ITREND = -1 in IN7. Store the file TREN for these later runs.
3. Perform an iterative procedure to converge on a solution as follows:
 - a. Run TREND to get OUI file.
 - b. Run INVERT to get OUTMOD, OUTBIN, and OUTCOV files.
 - c. In OUTBIN, if EBAR >1.0 for the desired solution, select the desired solution from OUTMOD (delete the rest of OUTMOD), change the name from OUTMOD to XMOD, and repeat from step a. Continue until EBAR \leq 1.0 or until EBAR no longer decreases.

Selecting a desirable solution in OUTMOD is a complex task because the list of solutions contains the unconstrained solution for different ALPHA values as well as the various constrained solutions. In addition, the selection of a model on which to perform the iterative procedure is subjective. The following discussion of problems that can occur with any solution can serve as a guideline for selecting a desirable solution.

During processes a through c in step 3 above, several problems can occur. Models with EBAR <1.0 may not exist. From this situation we can infer that the rectangular grid blocks are too large, or the data errors are underestimated, or the data are inconsistent. In the first few iterations, the depths of some blocks may be found to be negative. The statement of the problem indicates this is an impossibility for the final result. Nonlinearities in the system probably produced this result. Changing the negative depths to small positive depths, and optionally increasing the size of the stabilization factor, and then continuing to iterate will correct the situation.

Several features of the solution should be noted. In areas of high gravity-data density, the total error will be smaller than the *a priori* estimate; if so, the data improved on the estimate. In areas where the total error is close to the *a priori* estimate, the gravity data

provide little useful information about the depths; the total error, therefore, is equal to the *a priori* value. A large value for the resolving power of a depth estimate indicates a depth that cannot be resolved well at the given stabilization factor ALPHA. In areas of poor resolution, we rely on the initial model, not the data, to determine the depths. Areas of high gravity-data density show large, propagated data error, because the data are being used more extensively to calculate the parameters. INVERT provides resolution and correlation matrices of the depth estimates. To print these matrices, change IPRINT in line 1 of OUI from 0 to 1. The rows of the resolution matrix are the resolving kernels for each depth estimate. Good resolution implies a delta quality to the row values.

Solutions that have rapid oscillations (short wavelength features) in the depth estimates may be found. If these oscillations are geologically unreasonable, they can be suppressed in two ways. The stabilization factor ALPHA can be increased, thus forcing the inversion code to produce a solution closer to the initial model. If the initial model is without rapid oscillations, increasing ALPHA will produce smoother models. Positive correlations between depth estimates in the *a priori* depth-covariance matrix in IN6 can also be introduced. A nondiagonal, *a priori* covariance matrix with positive correlations will produce a smoother model because the *a priori* correlations effectively reduce the number of degrees of freedom available in the inversion scheme; thus, smoother models are obtained.

Special attention should be given to the size of the perturbations in the final solution to ensure that the final iteration does not exceed the region of local linearity. The resolving power technique of linear inversion theory is applicable to nonlinear problems that may be linearized around some approximate model, if the range of linearity is large enough. The required size of the region of linearity is a difficult question. Jackson⁴ proposes several tests on the linearity assumption; the final iteration should pass one of them.

After an acceptable solution has been found, AVERAGE will find the average and the standard deviation of the average of a selected set of depth estimates. AVERAGE can also calculate the difference and the error in the difference between two averages. If the grid spacing in

INVERT is too small to determine an individual depth adequately, the average of several depth estimates can give a useful estimate of the depth over the larger area. To determine and scope the presence of scarps or faults, the program can also calculate the mean difference between two sets of depth estimates.

AVERAGE is an interactive program that prompts the user. AVERAGE requires the file OUTCOV as input. INVERT automatically generates OUTCOV. The parameters are numbered in the same order as they appear in INVERT. The averages and the standard deviation of the averages are given in kilometers.

The program SEARCH helps formulate the input gravity files IN1 and IN2 from the NTS gravity data. From the NTS file HEALEYNTS, SEARCH selects gravity values for specified regions. The program is interactive and will ask for the E-W and N-S dimensions of an inner and an outer data block. The inner data block is the rectangular region whose gravity values are to be inverted into estimates of the depth to the basement. The outer data block is the rectangular region whose gravity values are used to calculate the regional trend. The user should specify these E-W and N-S dimensions in metres for the HEALEYNTS data file. The inner block should cover the entire region of interest for inversion; the outer block should extend for a considerable distance outside the inner block to define the regional gravity adequately. The user should apply common sense and prudence in specifying both sets of dimensions because the combination of the inner-data-block size and the size of the prisms in the model will largely determine the amount of computer core and central processing unit (CPU) time required. SEARCH generates output files IN1 and IN2 which, in name and format, are exactly what TREND requires as input.

FILE DESCRIPTIONS

INPUT FILES FOR TREND

The input files required for TREND are described below.

• IN1—(G(I), X(I), Y(I), I = 1, N) Format: (3F10.3)

where:

G = gravity value to be inverted (mgal)

X = X position in grid of gravity point 1 (m)

Y = Y position in grid of gravity point 1 (m)

These data are inverted to find the basement structure. SEARCH can generate this file for NTS data. This data set is not needed if ITREND = 2 in IN7.

- IN2—(GO(1), XO(1), YO(1), I = 1, NO) Format: (3F10.3)

where:

GO = gravity values to be used for regional trend removal (mgal)

XO = X position in grid of gravity point 1 (m)

YO = Y position in grid of gravity point 1 (m)

A least-squares plane is fitted through these gravity values for regional trend removal. The values predicted by the plane are subtracted from the data in IN1, if desired. If trend removal is not desired or trend removal information was previously calculated, then IN2 is not needed (i.e., when ITREND = -1 or 0 in IN7). SEARCH can generate this file for NTS data.

- IN3—WX, WY, COORDX, COORDY Format: (4F10.3)
 IWX(I), I = 1, NX Format: (8I10)
 IWY(I), I = 1, NY

where:

WX = width of unit block in rectangular grid in X direction
 (km)

WY = width of unit block in rectangular grid in Y direction
 (km)

COORDX = X position of center of block pattern in grid (km)

COORDY = Y position of center of block pattern in grid (km)

IWX = separation of x grid lines in terms of unit-block width
 WX

IWY = separation of y grid lines in terms of unit-block width
 WY

This data file is not needed if only trend removal information is desired (ITREND = 2 in IN7). These dimensions are illustrated in Fig. 1. Grid is automatically centered on the position (COORDX, COORDY).

- IN4--(RHO(I), I = 1, M) Format: (SF10.3)

where:

RHO = density contrast of blocks (gm/cm^3)

The density contrast is the difference (generally negative) between the sediment density and the basement density. The blocks are ordered from left to right (increasing X values) at constant Y values and then are repeated from left to right at the next higher Y-grid values (see Fig. 1). This data file is not needed if in IN7, ITREND = 2.

- IN5--(WORK2(I), I = 1, MM) Format: (8F10.3)

This file contains the covariance matrix of gravity data in IN1 (mgal^2). File IN5 has three storage modes:

- 1) Diagonal mode and all diagonal values are equal—ICE = -1 and MM = 1
- 2) Diagonal mode—ICE = 2 in IN7 and MM = N
- 3) Symmetric mode—ICE = 1 in IN7 and MM = (N*(N+1))/2

See Fig. 2 for an illustration of the data storage modes. This data file is not required if ITREND = 2 in IN7.

- IN6--(WORK4(I), I = 1 MM) Format: (8F10.3)

This file contains the *a priori* covariance matrix of block depths for which the gravity data in IN1 is being inverted (km^2). File IN6 has three storage modes:

- 1) Diagonal mode and all diagonal values are equal—IAPR = -1 and MM = 1
- 2) Diagonal mode—IAPR = 2 in IN7 and MM = M
- 3) Symmetric mode—IAPR = 1 in IN7 and MM = (M*(M+1))/2

See Fig. 2 for an illustration of data storage models. This data file is not required if ITREND = 2 in IN7.

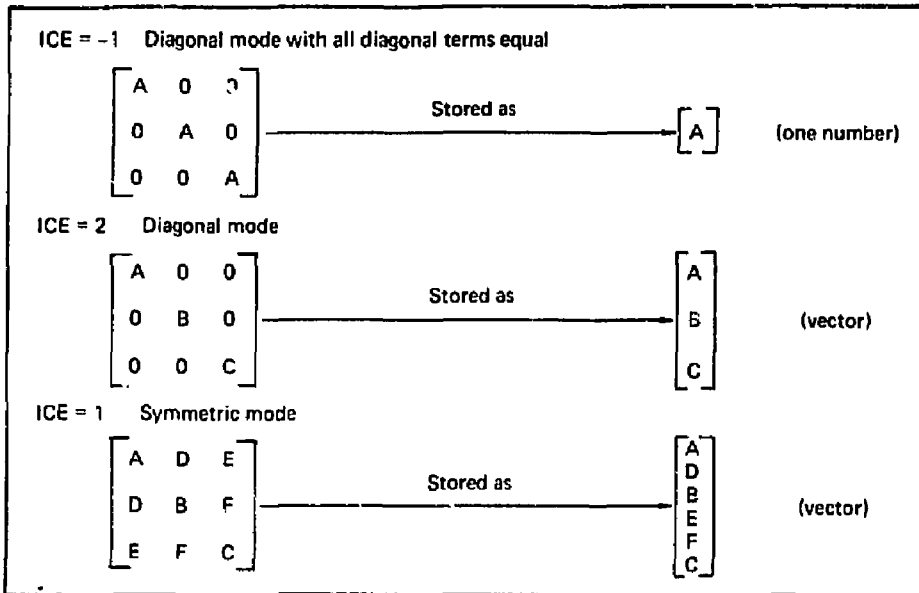


Fig. 2. Illustration of three storage modes for the covariance matrices.

● IN7—N, ITREND, NO, NX, NY, ICE, IAPR Format: (7110)

where:

N = number of gravity values in IN1

ITREND = -1 (regional trend removal from previous ITREND = 2 calculation)

= 0 (no regional trend removal)

= 1 (regional trend removal)

= 2 (regional trend removal information is calculated and stored in disk file TREN. ITREND = -1 uses data, stored in TREN, that was created by a previous calculation when ITREND = 2)

NO = number of gravity values in IN2 used for trend removal

NX = number of rectangular blocks in X direction in grid

NY = number of rectangular blocks in Y direction in grid

Total number of blocks M = NX * NY

ICE = -1 (diagonal mode with all diagonal terms equal in IN5)
= 1 (symmetric storage mode for IN5)
= 2 (diagonal storage mode for IN5)
IAPR = -1 (diagonal mode with all diagonal terms equal in IN6)
= 1 (symmetric storage mode for IN6)
= 2 (diagonal storage mode for IN6)

- XMOD—(XMODEL(I), I = 1, M) Format: (8F10.3)
The depths of the blocks define the initial model (km). The blocks are ordered like the density values in IN4 (see Fig. 1). This data file is not required if ITREND = 2.
- TREN—This data file is required if ITREND = -1. TREN is created by running TREND with ITREND = 2.

OUTPUT FILE FROM TREND

The output file produced by TREND is described below.

- OUI—This output data file produced by the program TREND is required as input to INVERT. Tape 42 is the logical input/output (I/O) number used in TREND to designate error messages from the program. Presently, TAPE42 = TAPE59 (TTY), so that errors are printed on the teletype.

INPUT FILES FOR INVERT

The input files required for INVERT are described below.

- OUI—The disk file OUI, generated by TREND, contains the following:
 - 1) N, M, IPUN, IPRINT
where:
N = number of data
M = number of parameters

ERROR MESSAGES

TREND may generate the error messages summarized in Table 1. The error messages that may appear in the output disk file OUTBIN from INVERT are summarized in Table 2.

TABLE 1. Summary of error messages that may be generated by TREND.

Message	Description
1. MATRIX INVERSION IN TREND NOT POSITIVE DEFINITE	Positions of gravity points in IN2 are probably in error. Check data format and ensure data are not repeated.
2. LOSS OF PRECISION IN TREND AT STEP	Loss of significant digits has occurred; result could give wrong results; size of problem could lead to round-off errors.
3. MATRIX NOT POS DEFINITE IN STAND DMFSD	The covariance matrix for revised gravity data formed from the covariance matrix for the original Bouguer gravity data and the covariance matrix for the trend removal is singular within the finite precision of the computer. Possible means of correction is to increase the size of the diagonal elements of the covariance matrix for the original gravity data. This increases the variance of each data point but reduces the correlations between data errors in the final covariance matrix. Also check to determine that data file IN5 is correct.
4. LOSS OF PRECISION IN STAND AT STEP xxx	Significant digits have been lost; current operation could give wrong results; size of matrix could lead to round-off errors. Possible means of correction is to increase the size of

TABLE 1. (cont.)

Message	Description
	the diagonal elements of the covariance matrix for the original gravity data. Check to determine that data file IN5 is correct.
5. ILLEGAL PARAMETER IN DMTDS IN STAND	A serious error in the input parameters has occurred. Check to determine that everything in data file IN7 is correct.
6. TRIANGULAR MATRIX IN DMTDS SINGULAR	The factored total covariance matrix for the data is singular. Possible means of correction is to increase the size of the diagonal elements of the covariance matrix for the original gravity data. Check to determine that data file IN5 is correct.

TABLE 2. Summary of error messages that may appear in the output disk file OUTBIN from INVERT.

Message	Description
1. XSTAND COVARIANCE MATRIX SINGULAR OR LOST PRECISION	<i>A priori</i> the covariance matrix is singular or close to being singular. To correct, check to determine if the input (in OUI) was really desired or change values in the <i>a priori</i> system.
2. ALPHA = xxxx NOT BIG ENOUGH, IER IN DSINV = xxx	The matrix $M = A^T A + \frac{2}{\alpha} I_m$ is singular with the set tolerance. To correct, increase the value of ALPHA.
3. $RM^{-1}B^T$ IS NOT POSITIVE DEFINITE xxx	The constraint matrix B is inconsistent, improperly entered, or singular. To correct, check to determine that B matrix is correct and that equations are neither repeated nor inconsistent.

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