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A scattered equivalent-source method for interpolation and gridding of potential-field data in three dimensions

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ABSTRACT

Potential-field geophysical data observed at scattered discrete points in three dimensions can be interpolated (gridded, for example, onto a level surface) by relating the point data to a continuous function of equivalent discrete point sources. The function used here is the inverse-distance Newtonian potential. The sources, located beneath some of the data points at a depth proportional to distance to the nearest neighboring data point, are determined iteratively. Areas of no data are filled by minimum curvature. For two-dimensional (2-D) data (all data points at the same elevation), grids calculated by minimum curvature and by equivalent sources are similar, but the equivalent-source method can be tuned to reduce aliasing.

Gravity data in an area of high topographic relief in southwest U.S.A. were gridded by minimum curvature (a 2-D algorithm) and also by equivalent sources (3-D). The minimum-curvature grid shows strong correlation with topography, as expected, because variation in gravity effect due to variation in observation-point elevation (topography) is ignored. However, the data gridded and reduced to a level surface at the mean observation-point elevation, by means of the equivalent-source method, also show strong correlation with topography even though variation in observation-point elevation is accounted for. This can be attributed mostly to the inadequacy of constant-density terrain correction or to data error. Three-dimensional treatment in this example is required as a means of calculating the data onto a level surface, above regions where data and geologic sources overlap, as a necessary first step for making geologic correction, variable-density terrain correction, and evaluating data error.

Better spectral estimates are obtained by direct calculation of the Fourier transform of the equivalent-source function than by the discrete fast Fourier transform computer algorithm.

Gridding is the Achilles' heel of potential-field geophysics.
M. Nabighian
Denver 1990

INTRODUCTION

We rarely interpret our data directly. Rather, we interpret shadows of our data as these data are reflected in values interpolated onto regular grids or profiles. Gridding embodies forgotten compromises made at an early stage of analysis from which we may suffer later on—an Achilles' heel.

Common compromises are these:

1) Data in 3-D space are gridded using 2-D algorithms.
2) For irregularly scattered point data, the grid interval is too small in some places and too large in others.
3) Algorithms struggle to fit the data, rather than the error envelope of the data.
4) For stream data (closely spaced measurements along widely spaced lines, as in airborne surveys), the severe anisotropy of the sampling is ignored.
5) The preceding problems could somehow be avoided and the interpolated grid still be unsatisfactory in areas of sparse control.

The method developed here primarily addresses irregularly spaced (scattered) data in three dimensions—items 1–3 above. It was developed for reduction of gravity data in areas of high topographic relief; the example treats gravity data from a very rugged volcanic terrain in the Rocky Mountains of southwest Colorado, USA.

Data in the example are decidedly 3-D, unevenly scattered, and probably contain errors. The new method allows the data to be calculated on a common level elevation datum and thereby offers a clear mathematical-theoretical advan-

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tage over conventional 2-D gridding by, for example, minimum curvature. Yet, in the practical example, differences in results by the two methods cannot be easily discerned. The problem is not only with the general mathematics of 3-D interpolation. Rather, the major problem has to do with the geology of near-surface variation in lithology and physical property. Therefore, the purpose of this paper is threefold: to describe a workable solution to the mathematical problem of calculating the data onto a common elevation datum; to show how the mathematical treatment exposes the geological problem; and to suggest that the mathematical treatment is indispensable in further analysis of data in rugged terrain.

DERIVATIONS: GENERALIZED EQUIVALENT-SOURCE MODEL

Dampney (1969) showed that a collection of n gravity values could be fit by calculating the gravity effect of n point masses ("equivalent sources"), one located directly beneath each data point. All point masses were at a common depth. The depth to the mass layer was assigned and the resulting linear system solved for the masses by inversion of an $n \times n$ matrix. Further effort has been directed to consideration of larger (von Frese et al., 1988) and larger and undetermined systems (Leão and Silva, 1989) and to finding the best depth to the grid of sources (Hansen and Miyazaki, 1984; and Xia and Sprowl, 1991). See Xia and Sprowl (1991) for a recent review. "Equivalent sources" has come to refer specifically to an ensemble of point masses on a common level or surface congruent with the observation surface, at least in the North American literature. Here, inasmuch as the sources are not necessarily masses and are not necessarily on a common level, I refer to these as "generalized equivalent sources," shortened to "equivalent sources," or just "sources."

Define the sequence of sources $\{c_n(\xi_n, \eta_n, \zeta_n)\}$ such that

$$\left| f_i(x_i, y_i, z_i) - \sum_{n=1}^{N} \frac{c_n}{\sqrt{(x_i-\xi_n)^2+(y_i-\eta_n)^2+(z_i-\zeta_n)^2}} \right| < \varepsilon, \tag{1}$$

where $\{f_i\}$ represents discrete data measured at $\{x_i, y_i, z_i\}$, with expected error ε, referred to a right-handed Cartesian system with the z (or ζ) axis down. The functional relationship has the form of a Newtonian potential with, for gravitational potential, $\{c_n\}$ being proportional to point masses at $\{\xi_n, \eta_n, \zeta_n\}$. Equation (1) could, however, be applied to any discrete set of potential-field data, inasmuch as the calculated field of the model (the summation term in 1) satisfies Laplace's equation and vanishes as $z \to \infty$. I use the potential in preference to first or second derivatives of the potential associated with, respectively, gravity and magnetic fields measured geophysically, because the potential is more general, computationally simpler and faster, and attenuates least with distance. The latter property of the potential is especially important in the case of a source distribution of discrete points.

Nonuniqueness guarantees many different ensembles of sources from which to choose. The task is to find a particular ensemble whose calculated field fits the data, interpolates smoothly between data points in three-dimensions, and can be arrived at efficiently in terms of computer time.

Working each time on the most anomalous data value, I will build up the ensemble iteratively. Assume, for ease of discussion, that I have already removed the mean value $\bar{f}$ from the data. I find the index of the largest value i_m, such that

$$|f_{i_m}| = \max\{|f_i|\}, \tag{2}$$

and for the first source, require that

$$f_{i_m}(x_{i_m}, y_{i_m}, z_{i_m}) = \frac{c_1}{\sqrt{(x_{i_m}-\xi_1)^2+(y_{i_m}-\eta_1)^2+(z_{i_m}-\zeta_1)^2}}.$$

Thus, one equation involving four unknowns: c_1, ξ_1, η_1 and ζ_1. Locate the source immediately beneath the i_mth data point, and the problem reduces to

$$f_{i_m} = \frac{c_1}{|z_{i_m} - \zeta_1|}, \tag{3}$$

leaving unknown only how deep to put the source. A deep source will produce smoother calculated fields [refer to equation (1)]. Too-deep sources, however, will not accommodate locally high-frequency response needed in areas where data points are tightly clustered. Recognizing that optimum equivalent-source depth and data density are related, we exploit this relationship by making source depth ζ_1 proportional to the distance between data point i_m and its nearest neighbor. Thus

$$\zeta_1 = a d_{i_m}, \tag{4}$$

where a is a proportionality factor to be decided by experiment, and

$$d_{i_m} = \min\{\sqrt{(x_{i_m}-x_n)^2+(y_{i_m}-y_n)^2+(z_{i_m}-z_n)^2}\}, \quad \text{all } n \neq i_m. \tag{5}$$

Evaluating equation (3) for c_1 gives us a complete definition of the first source:

$$\xi_1 = x_{i_m}$$

$$\eta_1 = y_{i_m}$$

$$\zeta_1 = a d_{i_m},$$

and

$$c_1 = f_{i_m}|\zeta_1 - z_{i_m}|.$$

Remove the effect of this source from all the data, forming

$$\{f_{i,2}\} = \left\{ f_{i,1} - \frac{c_1}{\sqrt{(x_i-\xi_1)^2+(y_i-\eta_1)^2+(z_i-\zeta_1)^2}} \right\};$$

find max $|f_{i;2}|$, fit a second source to it, and remove this and subsequent sources from $f_{i,n}$ until, after N' iterations, max $|f_{i;N'}| < \varepsilon$.

The sequence {max $|f_{i;n}|$} does not necessarily decrease monotonically with n. The process may not reach ε at all if a of equation (4) is chosen too large (making sources too deep), or if ε is too small. In practice, the sequence has been found to decrease robustly at first but will oscillate within a narrowing envelope. The associated computer program stops after either a specified number of iterations or when max $|f_{i;n}| < \varepsilon$, whichever comes sooner.

Suppose, after N' iterations that max $|f_{i;N'}| < \varepsilon$. We then have an ensemble of N' sources, the forward calculation of which [summation term of equation (1)] fits the data. There may be more or fewer sources than there are data points. Each source is beneath a data point at a depth proportional to the distance to that data point's nearest neighbor. There is not necessarily a source beneath every data point. Conversely, because all data points are repeatedly examined in an iterative process, more than one source may occur beneath a given data point. Inasmuch as all sources beneath a given data point must be at the same depth, these sources can be combined as one by superposition. After collapsing superimposed sources, we have an ensemble of $N < N'$ equivalent sources sufficient to fit the data.

The value of parameter a, which determines the source depth, can be selected by experiment, but in general we seek to put the source deep enough so that its gravity effect is smooth in the immediate neighborhood of the data point, yet diminishes rapidly at and beyond the neighbor point. The inflection point of the inverse-distance function [equation (1)] occurs at a horizontal distance 0.7 depth units from the source. Therefore a value of $a = 1.4$ in equation (4) puts the inflection point of the field of each source at the corresponding neighbor point, and this value was used in the example. A larger value of a, forcing sources deeper, can provide a sort of low-pass filter, as discussed below. In this system increasing the depth to the sources results in fewer sources (and poorer fit to the data points), and therefore does not amplify high-frequency noise, a problem discussed in Xia and Sprowl (1991) for a system having a fixed number of sources. Some experimentation with a may be required.

Aliasing of high-frequency signal due to undersampling is a severe problem in gridding potential-field geophysical data. The effect is rarely noticed in contour maps, but is obvious in high-gain filters such as shadowing or downward continuation. A gridding algorithm should, therefore, endeavor to fit the error envelope of the data, rather than the data themselves. It should undershoot locally very high data values, and overshoot locally very low values, to minimize aliasing of local fine structure. The equivalent-source method can attempt this objective if each source is fit not to f_{max} but to $f_{max} \pm \varepsilon$, as appropriate, thereby providing a means of nonlinear smoothing.

GRAVITY DATA IN LAKE CITY CALDERA

The San Juan Mountains in southwest Colorado is a complex Paleogene arc-magmatic complex (Lipman, 1976) containing multiple calderas. Gravity data used here are from the Lake City caldera, Colorado (Grauch and Campbell, 1985). The area is 25 by 32 km, within which elevations range from 2600 to 4700 m. Gravity data comprise 231 stations with elevations in the range 2630 to 4280 m (σ = 466 m). Survey specifications are detailed in Grauch and Campbell (1985), listing 280 gravity stations. Data used here were obtained on magnetic tape directly from Grauch. Her data set included some redundant stations, as often occur in combined data bases. After averaging stations within a 100 m radius, I analyzed 231 stations. Terrain-corrected Bouguer anomaly is based on a reduction density of 2.4 g/cm^3, determined by Grauch and Campbell by inspection of Bouguer anomaly maps. They estimate error due to elevation at 1 mGal and error due to terrain correction also at 1 Mgal. Several of the terrain corrections are over 30 mGal, and some do not include inner-zone correction. The estimate of terrain-correction error may be too low.

Topography of the Lake City area (Figures 1a and b) reflects an eroded caldera with scalloped rim, a resurgent central dome, and an intervening topographic moat. Figure 1a shows the geographic location of the area and actual topographic relief (over 2000 m). Figure 1b and subsequent shaded-relief grey-scale images are registered to Figure 1a but depict only relative amplitudes. All images in the subsequent figures are scaled linearly (not stretched, i.e.), and all depict illumination from the northeast. They were constructed using image software in Livo (1990).

Gravity stations are irregularly spaced with an average coverage of one station per 3.5 km^2. In the area of fairly detailed coverage, station spacing is about 1 km. I gridded the data on a 0.5 km grid by minimum curvature (Briggs, 1974) using the computer program developed in Webring (1981) and Godson and Mall (1989). Grid values range from -295.2 to -255.6 mGal, with an average value of -281.9 mGal and standard deviation of 6.9 mGal. The resulting map (Figure 2) is clearly correlated with the topography (compare Figures 1 and 2). Correlation with topography is to be expected because of the inappropriateness of a uniform reduction density, and because gravity stations in the valleys are closer to subcaldera features than are stations on the ridges. The so-called "free air" and "Bouguer" corrections applied to gravity data do not project gravity anomaly values onto a common elevation datum, as is sometimes erroneously supposed. In as rugged an area as this, one cannot say to what uniform elevation the field depicted in Figure 2 should be associated. Figure 2 depicts the result of a 2-D algorithm applied to 3-D data where, in addition, some of the stations are at a lower elevation than some of the disturbing masses, and therefore the regions of the data and the regions of the geologic masses overlap.

An ensemble of equivalent sources was fit to the Lake City gravity data by the proposed method. One thousand iterations on the 231 station data set took about 40 s on a 386/33 microcomputer. Convergence (Figure 3) was rapid at first but seemed constrained to a lower bound of about 1.3 mGal, starting from an initial value of 29.7 mGal. Parameter a was assigned a value of 1.4.

One thousand iterations were clearly too many (Figure 3) but were done to observe the process. A total of 141 sources (i.e., $N' = 1000$, $N = 141$ in the notation of the derivations) were required to fit the 231 gravity stations. Recalculated at the 231 data points, the maximum difference between the

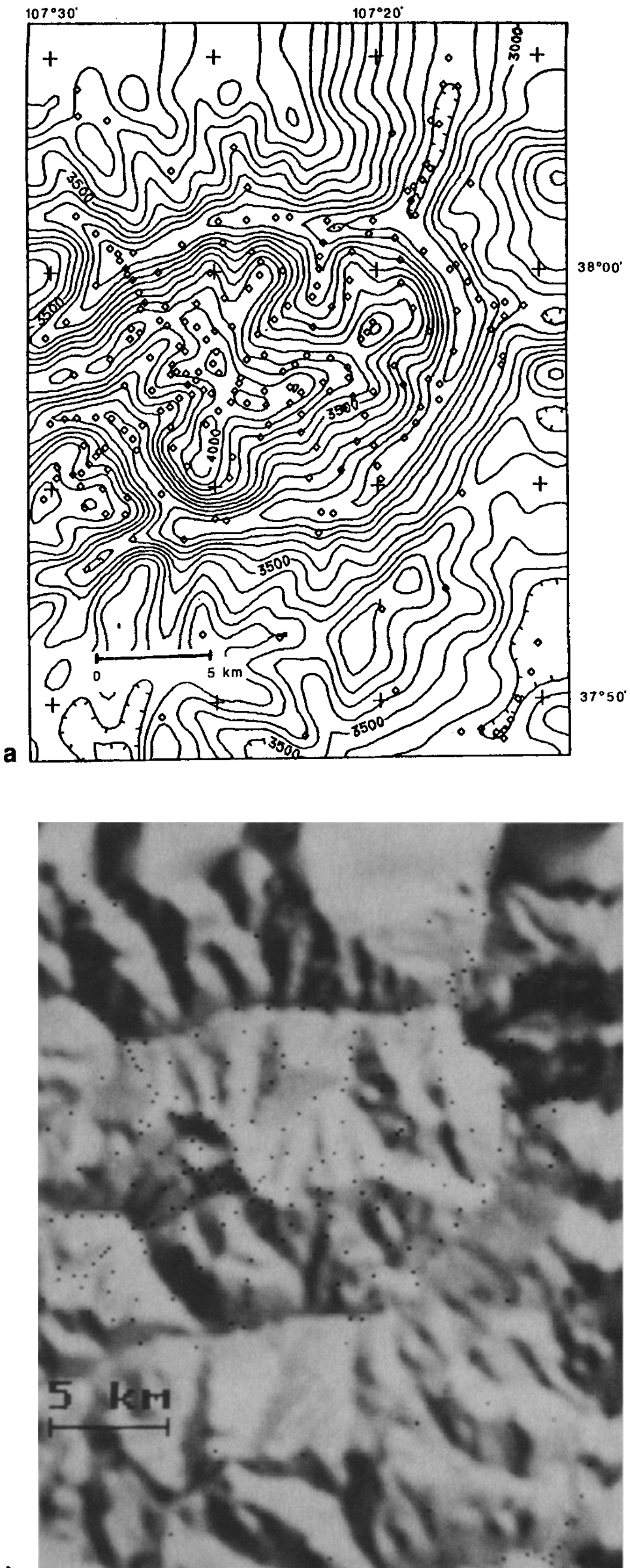

FIG. 1. (a) Topographic map of Lake City caldera showing gravity stations. Contour interval is 100 m. Coordinates are latitude and longitude. (b) Lake City topography shadowed from northeast; spots show gravity stations.

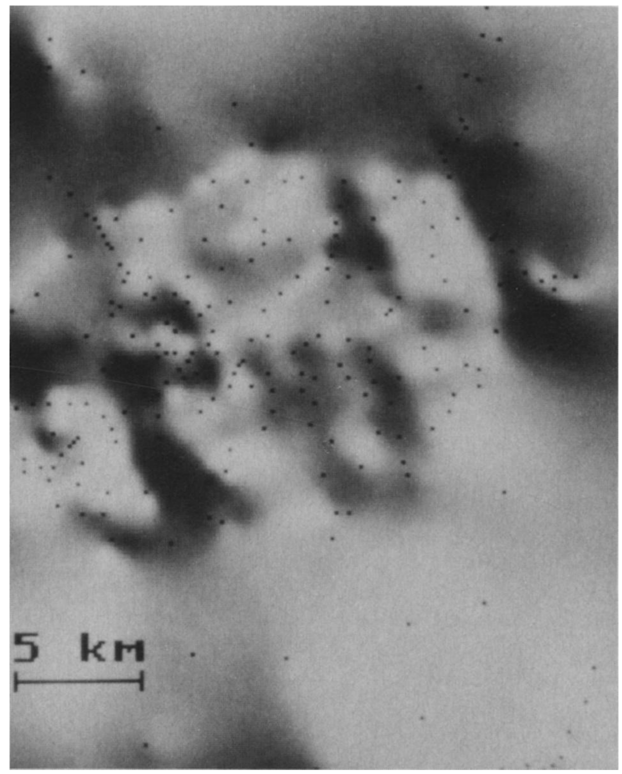

FIG. 2. Bouguer gravity anomaly gridded by minimum curvature.

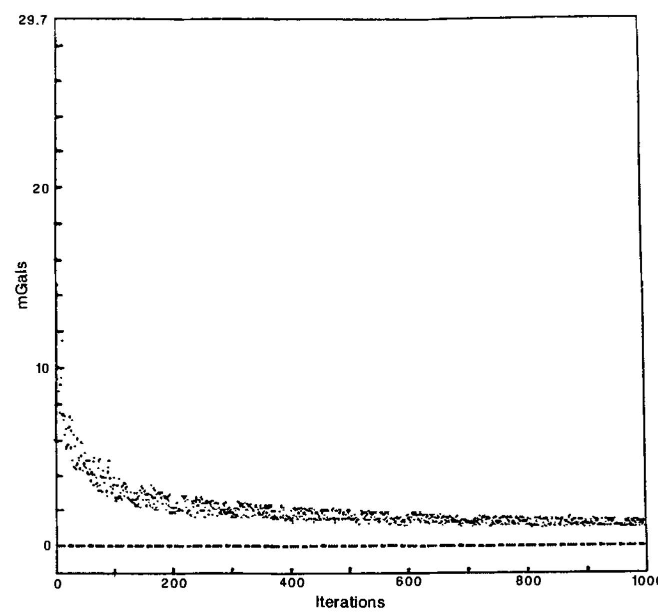

FIG. 3. Convergence graph showing largest residual error against iteration number.

actual and the calculated value (absolute value) among the 231 data values was 1.35 mGal; the mean was 0.15 mGal, and the standard deviation was 0.60 mGal. Recall that the algorithm, by design, undershoots local high station values or overshoots local low station values, to reduce the effect of aliasing.

Having obtained an ensemble of equivalent sources that fit the data we can proceed by forward calculation to effect a 3-D interpolation of the data onto nodes of a grid on a level surface at a specified elevation (Figure 4). This can only be done in areas of control however, because fields calculated from point sources sag toward regions having no data and, consequently, no sources (Xia and Sprowl, 1991). Field values were not calculated for grid nodes for which the distance from those nodes to the nearest measurement station exceed that station's distance to its nearest neighboring station. The area so masked (31 percent of the area, black area of Figure 4), was filled in by minimum-curvature grid values (from Figure 2), yielding the completed grid shown in Figure 5. The part of the field determined by equivalent sources (Figure 4) was calculated on a level surface at 3400 m, the average elevation of the data. Elevation associated with the grid determined by minimum curvature is not defined (data are tacitly assumed to be coplanar), but can be treated as the elevation of the data points in the immediate vicinity of the control.

By visual comparison with the result obtained by 2-D gridding using minimum curvature (Figure 2), the leveled grid (Figures 4 and 5) has only slightly less correlation with topography (compare Figures 2 and 4). There is less of the high-frequency dimpling associated with undersampling and aliasing. Careful inspection of Figures 1b, 2, and 4 reveals instances where use of 3-D interpolation and continuation of the data onto a common level has produced a smoother field with less obvious correlation with topography.

The discouraging result, however, is that, contrary to expectations, reduction to a common elevation datum has produced only nominal improvement. In the example, and very likely in general, the mathematical problem of 3-D interpolation is not, after all, the major problem. The major problem is geologic. Correlation between reduced gravity and topography persists because a constant reduction density, as used in the Bouguer and topographic corrections, cannot represent the range of surface densities encountered. An elevation range of 2000 m and a terrain correction of 30 mGal, as in the Lake City case, can account for as much as 10 mGal of variation in reduced gravity per 0.1 g/cm^3 error in reduction density!

COMPLETING THE EQUIVALENT SOURCES

Normally, gridding is accomplished at the stage represented by Figure 5. This field is, however, a hybrid of two algorithms and in the following I require a field completely determined by equivalent sources, even in areas of no data. For this purpose I created synthetic data from the grid-node values of the masked areas (blank areas of Figure 4) as filled in by minimum curvature (Figure 2). Elevation of the syn-

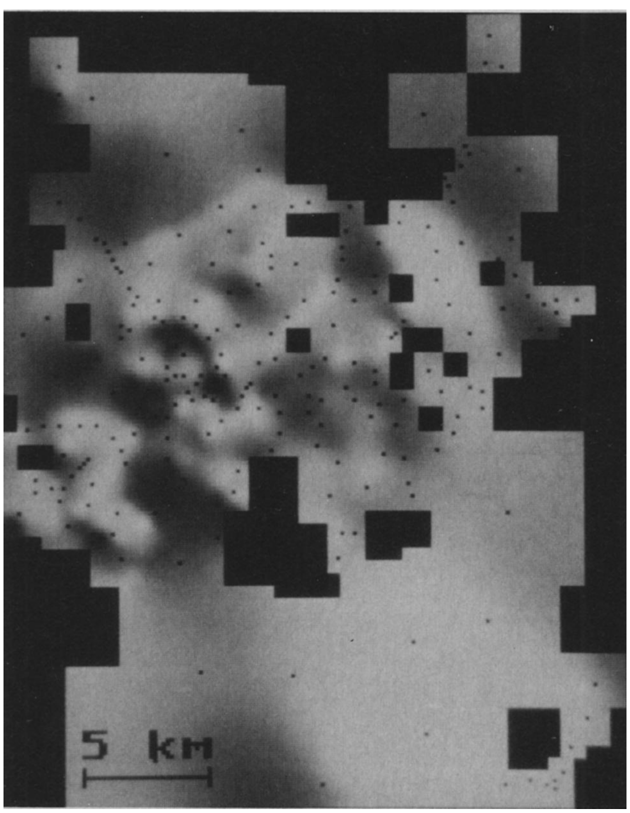

FIG. 4. Bouguer gravity anomaly gridded by equivalent-source technique; areas of no control are masked.

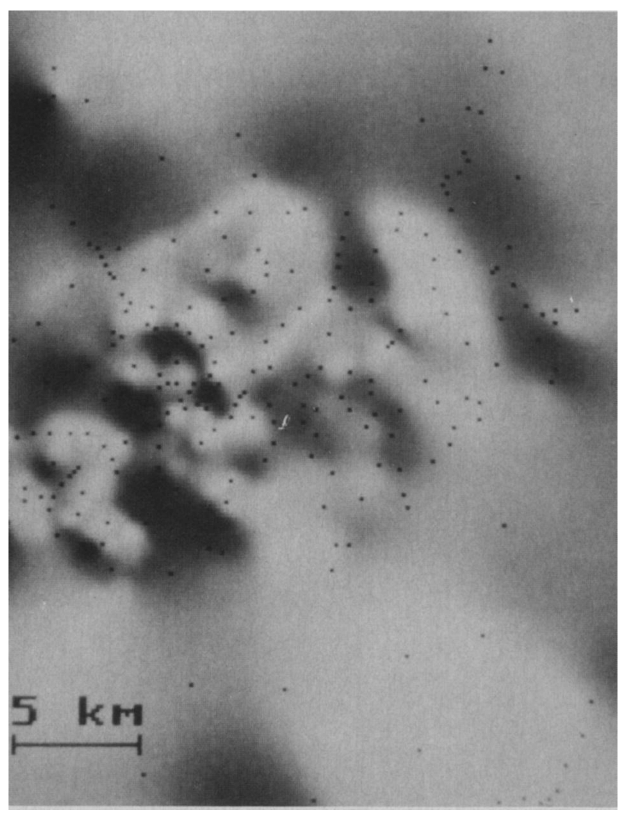

FIG. 5. Bouguer gravity anomaly gridded by hybrid of equivalent sources and minimum curvature.

thetic data was estimated from smoothed topography. The 1037 synthetic stations so obtained, combined with the original 231 actual stations, were used to achieve a field completely determined by equivalent sources. This field (not shown) is essentially identical to that of Figure 5. Only 209 sources were required to fit the total of 1268 original and synthetic data points. Fitted to the 1268 data points, the maximum error was 1.32 mGal; the mean error was 0.11 mGal, and the standard deviation was 0.36 mGal. Computer time to determine the sources and calculate the grid from the 1268 stations was about 2 minutes on a 386/33 microcomputer.

PSEUDO-AIRBORNE GRAVITY

Even after reducing the data to the average station elevation level, I find (Figures 1b, 2, and 4) the data *still* to be highly correlated with the topography. It is pointless, at best, to analytically continue data to any level below the highest station until a correction has been made for anomalous (with respect to the reduction density) geologic masses within the three-dimensional region occupied by the data themselves. The only practical method for making such a geological correction using standard modeling techniques requires as a first step that the data be continued onto a level *above* the geologic masses, in this case simulating airborne gravity. This can easily be done using the 209 equivalent sources obtained above. Only with the data represented on a level surface above all sources (here 4300 m, shown in Figure 6) are we prepared to further correct the data to account for local departure from the reduction density of 2.4 g/cm^3. The field shown in Figure 6 ranges from -289.2 to -260.8 mGal, with an average value of -281.6 and standard deviation of 4.7. Certain stations cause single-station spikes and are probably unusable. To judge from the strong correlation still remaining between gravity and topography (compare Figures 1b and 6), the reduced dynamic range caused by upward continuation, and the accumulating error chain, after geologic correction these data may provide few if any constraints on deep sources.

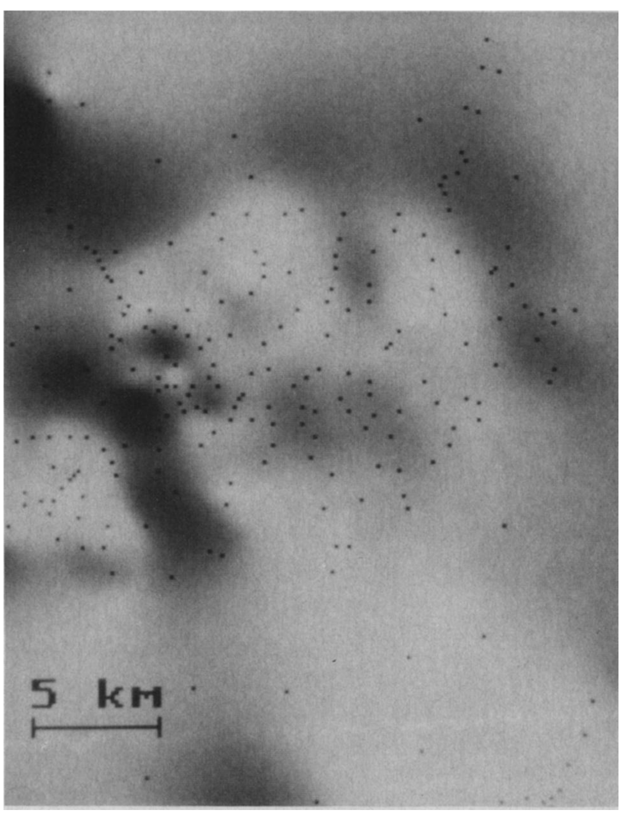

FIG. 6. Bouguer gravity anomaly calculated on 4300 m level by equivalent sources.

ANALYTICAL DISCRETE FOURIER TRANSFORM

The equivalent-source distribution also provides an alternative method of calculating Fourier spectra analytically. For comparison, I first calculated the discrete complex Fourier transform and its scalar amplitude spectrum (Figure 7) of the minimum-curvature grid (Figure 2) with the aid of a fast Fourier transform (FFT) algorithm for microcomputers (Hildenbrand, 1983; Godson and Mall, 1989). The grid was preconditioned by detrending and tilting it after detrending to make the southeast and northwest corners equal, then extrapolating the data to the north and east using a cosine taper to make opposite sides of the data wrap smoothly in both directions (unpublished computer program). This preconditioning significantly minimizes the distortion of the high-frequency and axial regions of the spectra, characteristic of the discrete transform, discussed in Cordell and Grauch (1982).[1]

Distortion and other problems with the discrete transform might be circumvented by calculating the Fourier transform directly from the equivalent sources. The continuous integral Fourier transform (see, for example, Bhattacharyya, 1967) of the nth point-source element [equation (1)] is

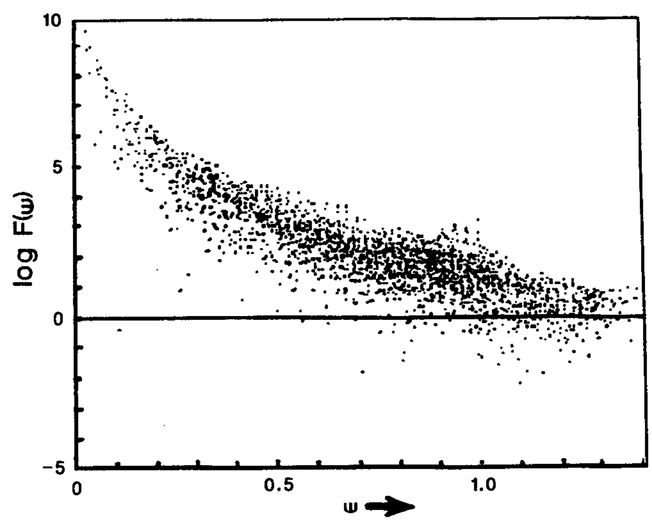

FIG. 7. Fourier amplitude spectrum of minimum-curvature grid by FFT.

[1] I refer to frequency rather than wavenumber in the space domain because frequency has units (km^{-1}) whereas wavenumbers do not, and because reference to the recurrence frequency of a given number of cycles/km is permissible English.

$$\frac{c_n e^{2\pi\omega(z - \zeta_n)}}{\omega} e^{-2\pi i(v_x \xi_n + v_y \eta_n)}, \tag{6}$$

where

$$i = \sqrt{-1}$$

(v_x, v_y) and (x, y) are transform pairs, and

$$\omega = \sqrt{v_x^2 + v_y^2}.$$

As a result, we can estimate a band-limited discrete transform by redefining

$$\xi_x \text{ as } \frac{j_x}{J_x \Delta x}$$

and

$$\eta_y \text{ as } \frac{j_y}{J_y \Delta y},$$

where

$$J_x = \text{number of columns}$$

$$J_y = \text{number of rows},$$

$$\Delta x, \Delta y \text{ are the grid intervals},$$

and

$$j_x \text{ and } j_y \text{ are integers}.$$

The discrete Fourier transform (Figure 8) was calculated on $z = -3400$ m from the 209 equivalent sources used to create the field shown in Figure 5. The transform derived analytically from equivalent sources is similar in the lower frequencies to that derived by FFT of the minimum-curvature grid (compare Figures 7 and 8). Their difference near the Nyquist (highest) frequencies reflects greater contamination in the minimum-curvature, FFT-based transform, as expected. These severely inhibit high-gain filters such as downward continuation (Cordell and Grauch, 1982).

In midrange, the analytical equivalent-source transform seems *worse* than the FFT. This only reflects the fact that the equivalent-source transform incorporates the additional step of continuing some of the data downward through geologic sources onto the mean station elevation level (3400 m). It is fallacious to do this without prior geologic correction, as already discussed.

If we evaluate the equivalent-source transform on the "airborne gravity" level (4300 m, as in Figure 6) we would see the well-known exponential dampening of the spectrum due to upward continuation. Instead, to illustrate the role of parameter a of equation (4), I show (Figure 9) the transform evaluated on the 3400-m level for equivalent sources determined as before except that $a = 3.0$ instead of 1.4. In this case, 216 sources were required. Recalculated at the data, maximum error was 3.6 mGal, mean error was 0.8 mGal, and standard deviation was 1.9 mGal. The effect of increasing the value of a is to apply a linear low-pass filter akin to upward continuation. Figure 9 shows that this set of sources may miss high-frequency elements of the data related to uncorrected geologic-topographic effects, and thereby provide a cleaner spectrum.

DISCUSSION

Equivalent sources provide a 3-D interpolator having the useful properties of: (1) accommodation of variable data density; (2) a basis for analytical calculation of the Fourier transform; (3) linear and nonlinear smoothing; and (4) retention of single-point anomalies rather than smearing these so that bad data points escape notice. Calculation of the sources is fast, although the complete procedure is probably overly cumbersome unless some of its special properties are needed.

Ironically, where topographic relief is sufficient for three-dimensional interpolation to be a problem, we are likely to find shallow geology to pose proportionately an even greater

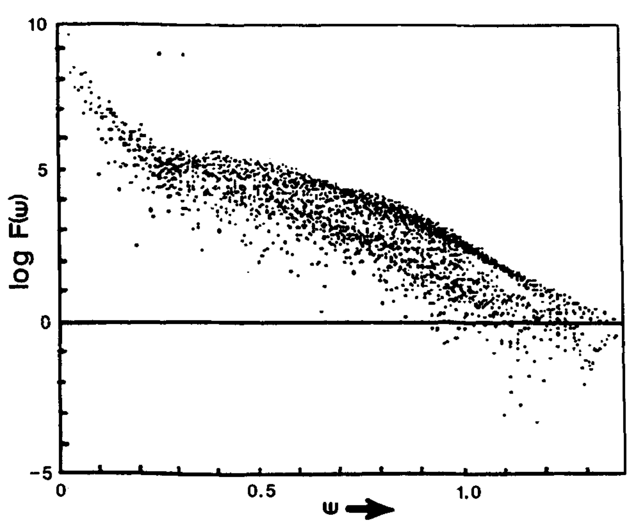

FIG. 8. Fourier amplitude spectrum calculated analytically from equivalent sources.

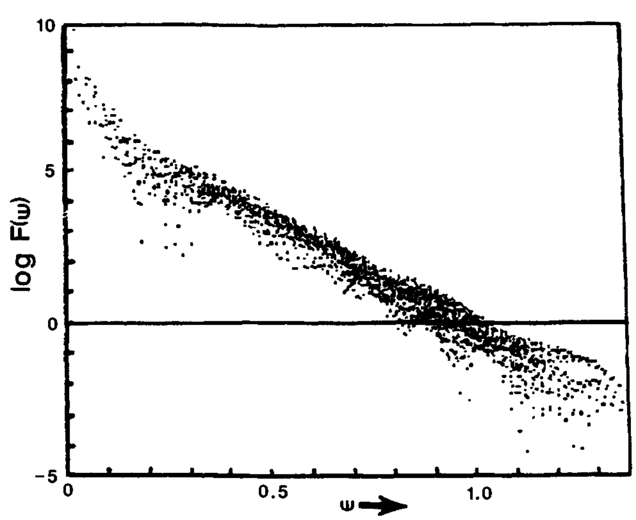

FIG. 9. Fourier amplitude spectrum calculated analytically from equivalent sources, $a = 3$.

problem. We cannot proceed until we have calculated the data onto a level above the topography.

Throughout this paper, I have contrasted equivalent sources favorably against minimum curvature. I do not disparage minimum curvature; it is probably the best algorithm for gridding almost all scattered-point geophysical data—the topographic relief in the Lake City example is extreme. Extreme topographic relief is found in a significant part of the Earth's and other planetary surfaces, however, and in these areas three-dimensional interpolation is required to get the data "pseudo-airborne" above the geology. Interpretation of the Lake City data would be perilous without it.

Geophysical distributions differ, and no one interpolator is suited to all. Neither minimum curvature nor equivalent point sources are appropriate for flight-line data, for example, because neither method explicitly exploits or even addresses the extreme anisotropy of flight-line data. The important consideration is that the interpolator accommodates the texture and dimensionality of the data, separate regions of data from regions of geologic sources, and smoothly fit the error envelope of the data, rather than the data themselves.

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