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Gravity field continuation of irregularly spaced data using least squares collocation

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SUMMARY

The calculation of Bouguer anomalies in high mountains requires a gravity field continuation from irregularly spaced gravity data on the topography to an equipotential surface. Least squares collocation (LSC) is successfully used for geodetic purposes and offers an elegant solution to this problem. A great advantage of this method is the possibility to give estimates of the accuracy of the approximated gravity field.

Of central importance in LSC is the covariance function. The influence on the result of the model covariance function (MCF), which replaces in the calculation the empirical covariance function (ECF) of the data, is studied. The synthetic model used for these studies is as realistic as possible, including topography, data gaps and noise. The quality of the predicted error seems to be much more sensitive to the choice of the MCF than the quality of the approximation. The improvement of the field continuation to an equipotential surface compared to simple interpolation is remarkable. An example of such a field continuation is given. The Bouguer anomaly in the Andes of northern Chile is continued to the sea-level by the combined application of collocation and simple models, describing regional parts of the gravity field.

Key words: station complete Bouguer anomaly, true complete Bouguer anomaly, field continuation, collocation, covariance function

INTRODUCTION

The approximation normally made, that the free air reduction with the normal vertical gradient reduces the measured gravity from the station-level to a certain reference-level (in most cases the sea-level) is not valid in high mountainous areas. In this case the effect of the anomalous vertical gradient can lead to errors which are not negligible. Model calculations in the Andes in South America (Götze *et al.* 1988) showed that for the Bouguer anomaly at a height of about 4000 m the effect can amount to 15 mGal! Considering the free air reduction Δg_{far} without approximation it appears that it is nothing more than a correction of the normal gravity at sea-level γ_0 to the station-level γ_{st} (Ervin 1977):

$$\Delta g'' = g_{\text{abs}} - \underbrace{(\gamma_0 + \Delta g_{\text{far}})}_{\gamma_{\text{st}}} + \delta g_{\text{top}} + \delta g_{\text{Bou}}, \tag{1}$$

where $\Delta g''$ is Bouguer anomaly, g_{abs} is the absolute gravity at the station (measured), γ_0 is the normal gravity at zero-level, Δg_{far} is the free air reduction (normal vertical gradient), δg_{top} is the topographic reduction, δg_{Bou} is the Bouguer reduction, and γ_{st} is the normal gravity at station level.

The subtraction of γ_{st} from the absolute gravity g_{abs} has no influence on the height of the station, so that Bouguer anomalies calculated in the classical way according to equation (1) have to be considered as station related. Tsuboi (1965) calls a Bouguer anomaly of this type *station Bouguer anomaly* in contrast to the *real Bouguer anomaly,* which is reduced to a certain reference-level. According to Granser (1982) I will use in the following the abbreviations SCBA (station complete Bouguer anomaly) and TCBA (true complete Bouguer anomaly). The calculation of the TCBA requires a field continuation of the SCBA which consists of irregularly spaced data which are not on an equipotential surface. Normal field continuation techniques, e.g. FFT (Degro 1986), are not suitable for this purpose, because they require input data on a regular grid all at the same height. The first attempt to solve this problem was given by Dampney (1969) with the equivalent source technique. Other solutions may be based on functions with limited spectra, the sin $(x)/x$ method and Fourier series (see e.g. Granser 1982).

As another solution to this problem, least-squares collocation (LSC) appears to be a powerful technique. A great advantage of LSC is the possibility to give an estimate of the error of the predicted gravity values. This method has been successfully used in geodesy for some years, but up to now it is not very common in geophysics.

THEORY

This section will state and briefly explain the fundamental formulas of collocation as they are needed for field continuation of gravity data. An extensive treatment of this theory can be found in Moritz (1980).

A main condition for the application of collocation is that the treated gravity field is a homogeneous and isotropic stochastic process. This condition is at least discussable. Nevertheless, if known regional features, e.g. trends, and the topographic-isostatic part of the gravity field are treated separately, as in the example of the gravity anomaly of the Andes given later, in my opinion this formalism may be applied. These problems are also discussed in Moritz' textbook.

Let $\mathbf{g}$ be the vector of n gravity values g_i. The formula for the predicted gravity $\tilde{g}_p$ at point p is:

$$\tilde{g}_p = \mathbf{C}_p^T \cdot \mathrm{C}^{-1} \cdot \mathbf{g}. \tag{2}$$

The elements c_{ij} of the $n \times n$ matrix C and the c_{pi} of the n-element vector $\mathbf{C}_p$ result from the covariance function of the gravity field $C(\psi, r, r')$;

$$c_{ij} = C(\psi_{ij}, r_i, r_j)$$

$$c_{pi} = C(\psi_{pi}, r_p, r_i),$$

where ψ_{ij} is the spherical distance between points i and j, ψ_{pi} is the spherical distance between points p and i, and r_i, r_j and r_p are the distances between earth's centre and points i, j and p.

The point p and the locations of the gravity stations may be at different heights. That means that gravity field continuation of data at different heights is possible by equation (2) in regions where the Laplace equation is valid. An estimate of the error of the predicted value $\tilde{g}_p$ is given by:

$$\tilde{\varepsilon}_p^2 = C(\psi = 0, r_p, r_p) - \mathbf{C}_p^T \cdot \mathrm{C}^{-1} \cdot \mathbf{C}_p \tag{3}$$

The gravity field defined by $\tilde{g}_p$ is harmonic for functions $C(\psi, r, r')$ satisfying the Laplace equation. The measured values are reproduced exactly. Observing that the measured values g_i are erroneous with a standard deviation d_i leads to the following formulas:

$$\begin{aligned} \tilde{g}_p &= \mathbf{C}_p^T \cdot \bar{\mathrm{C}}^{-1} \cdot \mathbf{g} \\ \tilde{\varepsilon}_p^2 &= C(\psi = 0, r_p, r_p) - \mathbf{C}_p^T \cdot \bar{\mathrm{C}}^{-1} \cdot \mathbf{C}_p \end{aligned} \tag{4}$$

where

$$\bar{c}_{ij} = c_{ij} \qquad i \neq j$$

$$\bar{c}_{ii} = c_{ii} + d_i^2.$$

In this case $\tilde{g}_p$ reproduces the measurements g_i only within the error d_i. The better conditioning of the matrix $\bar{\mathrm{C}}$ is a positive side effect of adding d_i to the main diagonal elements of C.

THE COVARIANCE FUNCTION $C(\psi, r, r')$

The covariance function $C(\psi, r, r')$ is of central importance in the above mentioned formulas. In the following section some of the fundamental characteristics of the covariance function are presented. First, pure interpolation is assumed,

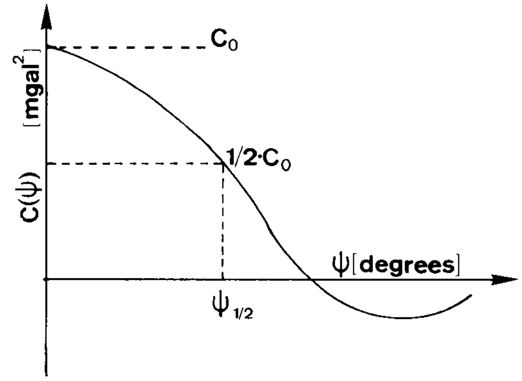

Figure 1. Typical covariance function of a gravity anomaly. C_0, Variance; ψ, spherical distance; $\psi_{1/2}$, correlation length.

i.e.

$$C(\psi, r, r') = C(\psi) \quad (r = r' = \text{const}).$$

Figure 1 shows a typical example of a covariance function. $C(\psi)$ for $\psi > 0$ is the mean value of the product of two anomalies within a spherical distance of ψ. $C(\psi) > 0$ means therefore that two anomalies at this distance are positively correlated, whilst for $C(\psi) < 0$ the correlation is negative. $C(\psi)$ approaches 0 for great ψ, since no correlation exists any more.

For the general case of $r \neq r'C$, (ψ, r, r') is the correlation between the gravity field at a radius r and the gravity field at a radius r'. Its general form is:

$$\begin{aligned} C(\psi, r, r') &= \sum_{n=2}^{\infty} k_n (n-1)^2 \left(\frac{R^2}{rr'}\right)^{n+2} \cdot P_n(\cos\psi) \\ &= \sum_{n=2}^{\infty} c_n P_n(\cos\psi) \end{aligned} \tag{5}$$

$$\cos(\psi) = \sin\theta \sin\theta' + \cos\lambda \cos\lambda' \cos(\lambda - \lambda')$$

where (r, θ, λ), (r', θ', λ') are spherical coordinates of two points, R is the mean earth radius, and P_n are the Legendre polynomials.

The terms for $n = 0, 1$ are missing, since the origin of coordinates is at the earth's centre of gravity and the mean value of all anomalies is equal to zero.

In order to apply collocation, the empirical covariance function (ECF) of the measured data at a mean station-level has to be determined first and a sequence c_n must be chosen so that the resulting model covariance function (MCF) $C(\psi, r, r')$ agrees with the ECF at the mean level as closely as possible. Further, c_n should be chosen in such a way that a closed expression is obtained for the sum in equation (5). Examples of such closed expressions with 2, 3 or more free parameters can be found in Tscherning & Rapp (1974) and Jordan & Heller (1978), for example.

THE SELECTION OF THE 'CORRECT' MCF

The ECF of the measured data can be derived from the following process, in which the data are assumed to be reduced by the mean value if it is not equal to zero:

(i) Creation of m distance classes of suitable size with $\psi_{i-1} < \psi < \psi_i$, $i = 1, \ldots, m$, $\psi_0 = 0$.

(ii) Search for all point combinations which belong to a certain distance class.

(iii) Calculation of the mean value of the product of all point combinations of one class.

(iv) The mean value of class i is assumed to be representative of the covariance function at the distance $\frac{\psi_{i-1}+\psi_i}{2}$.

(v) $C(0)$ is derived as the mean value of the anomaly squares.

(iv) Interpolation between the nodal points ψ_0, $\frac{\psi_{i-1}+\psi_i}{2}$, $i = 1, \ldots, m$ (for example with spline functions).

The calculated ECF is an approximation of the true covariance function at a mean station-level. For a very irregular station distribution it may be useful (only for the calculation of the ECF!) to interpolate the data in advance onto a regular grid by means of a simple process. A suitable MCF is then found by the following iterative procedure:

(1) Calculation of the ECF of the measured data.

(2) Search for a MCF which approximates as closely as possible the ECF on the mean station-level (for example, by variation of two free parameters in Jordan and Heller's function).

(3) Calculation of the gravity anomaly at a constant height by collocation, using the MCF found after step (2) taking the station height into consideration.

(4) Calculation of the ECF of the anomaly calculated in step (3).

(5) Search for a MCF for the ECF in (4).

Steps (3) to (5) are then repeated until the discovered parameters of the MCF are no longer significantly altered. The variance $C(0)$ and the correlation length $\psi_{1/2}$ are often used as the criterion for the adjustment of the MCF. The curvature at $\psi = 0$ and the position of the turning point are sometimes used as well (Moritz 1980; Kraiger 1987).

DATA SELECTION

The inversion of the $n \times n$ matrix $\tilde{C}$ is a further important problem in the application of collocation. As $\tilde{C}$ is full, it is difficult to deal with numerically for a large number of stations n. For this reason it is often imperative to make a suitable choice from the mass of measured data. Stepwise collocation presents an elegant solution to this problem (Moritz 1980):

(1) Selection of n measured values evenly distributed over the area of investigation.

(2) Creation of the $n \times n$ matrix $\tilde{C}$ and its inverse $\tilde{C}^{-1}$.

(3) Calculation of the gravity at all points which have not yet been included in $\tilde{C}$ and comparison with the values g_i.

(4) Search for m points at which the deviation is greatest.

(5) Creation of the $(n+m) \times (n+m)$ inverse including the m new points from (4).

Steps (3) to (5) are then repeated until a sufficient fit to the measured data is obtained. In the calculation of the new $(n+m) \times (n+m)$ inverse in equation (5), knowledge of the $n \times n$ inverse can be exploited. To avoid ill-conditioning the m points for the extension of the matrix are chosen so that the shortest distance between them exceeds a prescribed minimum. This method of stepwise collocation was successfully applied to the calculation of the geoid from vertical deflections in Austria (Sünkel 1983). Kraiger (1987) showed that numerical instabilities due to close points can also be avoided by a good choice of the curvature of the MCF at $\psi = 0$.

APPLICATION TO A SYNTHETIC MODEL

Using a synthetic, but as realistic as possible, gravity anomaly, this section will show the dependence of the result of collocation on the choice of the MCF during field continuation and illustrate how quickly the proposed iterative process for the determination of the MCF can supply a reliable result.

The synthetic model was created with 121 point masses at a depth of 50 km. The mass of these points was determined by a random number generator and was normalized so that an anomaly of about 50 mGal was obtained. The addition of noise with a variance of 0.25 mGal^2 leads to an anomaly that already looks quite realistic (Fig. 2).

In order to test the field continuation of irregularly distributed data by collocation, this anomaly was calculated over the topography shown in Fig. 3 with station heights between 750 and 4500 m. Then, by a random number generator, 200 of the originally 441 stations were selected in order to simulate data gaps as well. Figure 4 shows this anomaly with simple linear interpolation.

The ECF of the synthetic anomaly attains a variance of 117 mGal^2 and a correlation length of 0.44° (Fig. 5). With $C_0 = 114$ mGal^2 and $\psi_{1/2} = 0.46°$, however, only minimal deviations from the estimated values at 0 m level are

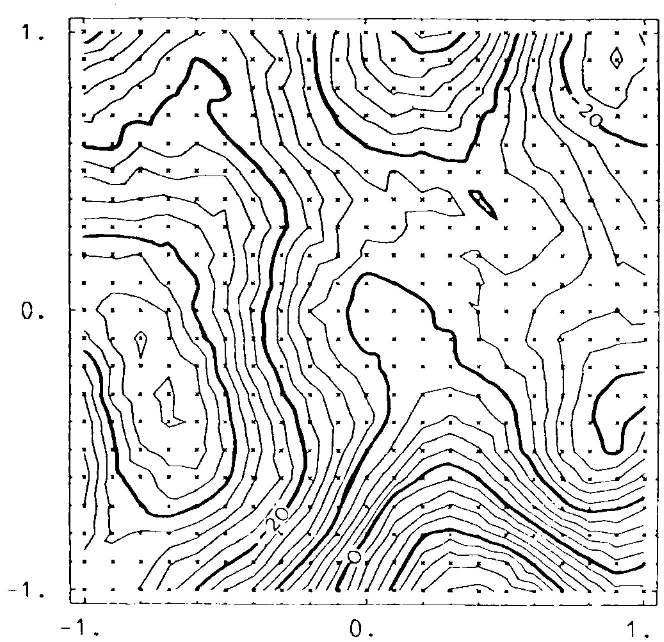

Figure 2. Synthetically generated gravity anomaly at sea level in the range −1° to +1° longitude and −1° to +1° latitude, with noise. Number of stations (x), 441; isoline interval, 2 mGal.

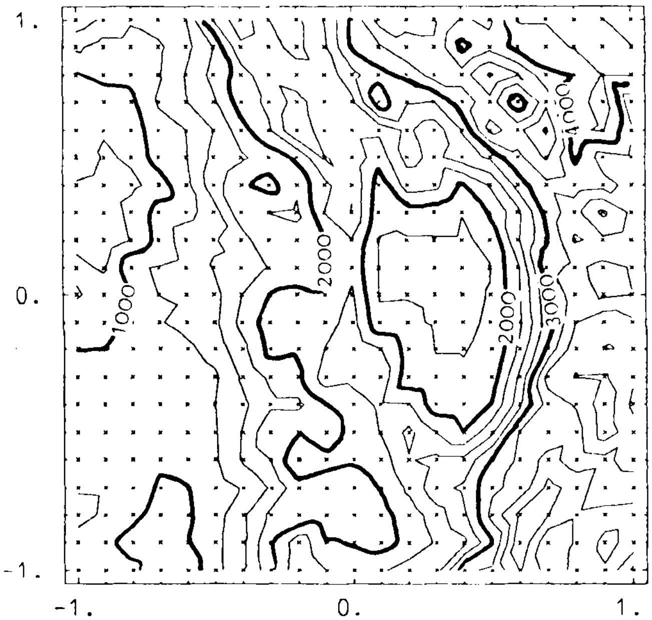

Figure 3. Topography of the 'survey area'. Isoline interval, 250 m.

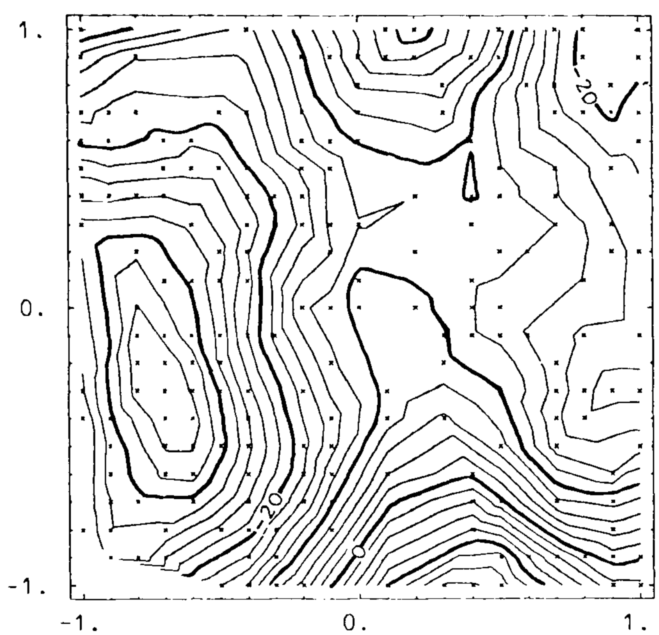

Figure 4. Synthetic anomaly calculated on the topography in Fig. 3 in simple linear interpolation. Number of stations (x), 200; isoline interval, 2 mGal.

observed for the 200 data on the topography (Fig. 4):

	C_0(mGal^2)	$\psi_{1/2}$
441 data at 0 m level	117	0.44°
200 data on the topography	114	0.46°

In order to be able to evaluate the effect of a completely wrong choice of MCF on the results, the collocation was carried out with three different functions after Jordan & Heller (1978) which I will call model N, S and L:

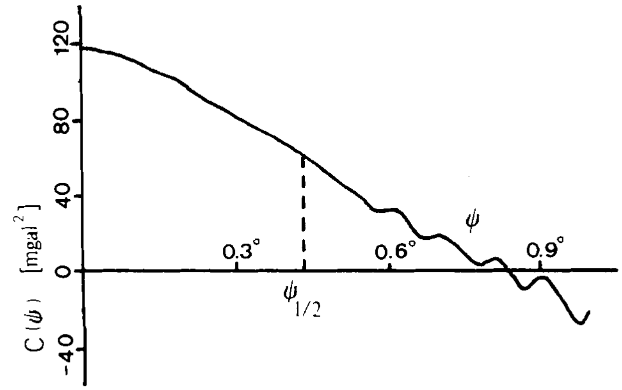

Figure 5. ECF of the synthetic anomaly in Fig. 2.

	C_0(mGal^2)	$\psi_{1/2}$
model N	117	0.44°
model S	117	0.24°
model L	117	0.87°

The variance C_0 was correctly chosen for all three models, since the variance can simply be changed by a factor in the MCF and since this factor has only a small influence on the result of the collocation after equation (4) for $\bar{g}_p$. The error estimation is admittedly influenced by C_0; it will be shown, however, that the anomalies calculated with the models S and L also reproduce the variance and correlation length fairly exactly, so that the error estimate could be improved with just one extra step in the proposed iterative procedure.

Using stepwise collocation 96 stations were chosen from the initial set of 200 stations (Fig. 4). The error of the measurements d_i was assumed to be 0.5 mGal, and thus conformed with the added noise. From these 96 stations on the topography the gravity anomaly was continued to zero-level and compared with the corresponding synthetic values at all 441 stations to show the quality of the continuation and the error estimation as well as the dependence of the result on the MCF. The same was done with the gravity field continuation to 10 km level. The results are shown in Table 1.

Results of the field continuation to 0 m level (Table 1)

The mean error $\bar{F}$ is caused mainly by a regional portion of the gravity field which was not taken into account by the data in the survey area. Even the 'wrong' MCF L gives a clearly better result than MCF N, since it (by choice) better approximates the anomaly outside the survey area (see below).

The standard deviation F of 0.55 mGal for model N (Fig. 6) is only slightly greater than the added noise of 0.5 mGal and is much better than for the models S and L. Even so it was still possible to correctly estimate the ECFs C_0 and $\psi_{1/2}$ with the gravity field by these completely wrong models! Thus, as already mentioned, a further step in the iterative procedure suggested above turned out to be successful in spite of the bad initial conditions.

A badly chosen MCF has a much clearer effect on the estimated error after (4) than on the standard deviation F.

Table 1. Results of the field continuation.

	$\bar{F}[mGal]$	F[mGal]	P[%]	$C_0[mGal^2]$	$\psi_{1/2}$
0 m level					
MCF N	-0.37	0.55	73.5	118	0.44°
MCF S	-0.54	0.97	91.2	119	0.44°
MCF L	-0.23	1.26	18.1	112	0.46°
10 km level					
MCF N	0.95	0.40	72.6	66	0.51°
MCF S	1.20	0.77	73.0	42	0.30°
MCF L	0.49	0,67	31.3	87	0.94°

$\bar{F}$, mean error } compared with noise free data at 0 m level.
F, standard deviation }
P, percentage of real errors within the estimated standard deviation.
C_0, $\psi_{1/2}$, ECF of the calculated anomalies.

Whilst P for MCF N is close to the theoretical value of 68 per cent, the error estimated with MCF L is much too large, with MCF S much too small.

Results of the field continuation to 10 km level (Table 1).

The mean error $\bar{F}$ behaves in a similar manner as in the downward field continuation and can be explained in exactly the same way. However, this time there is of course a different sign.

The standard deviation F for model N (Fig. 7) can be described as excellent at only 0.40 mGal just as can the error estimate at 73 per cent.

It is very interesting to compare the ECF of the synthetic anomaly at 10 km level ($C_0 = 71$ mGal^2, $\psi_{1/2} = 0.48°$) with the ECFs estimated after collocation using the MCFs N, S and L; model N shows excellent conformity even here.

BEHAVIOUR OF COLLOCATION OUTSIDE THE SURVEY AREA

This section will investigate the question, why the mean errors of the field continuation are relatively large and why the MCF L supplies a clearly better result.

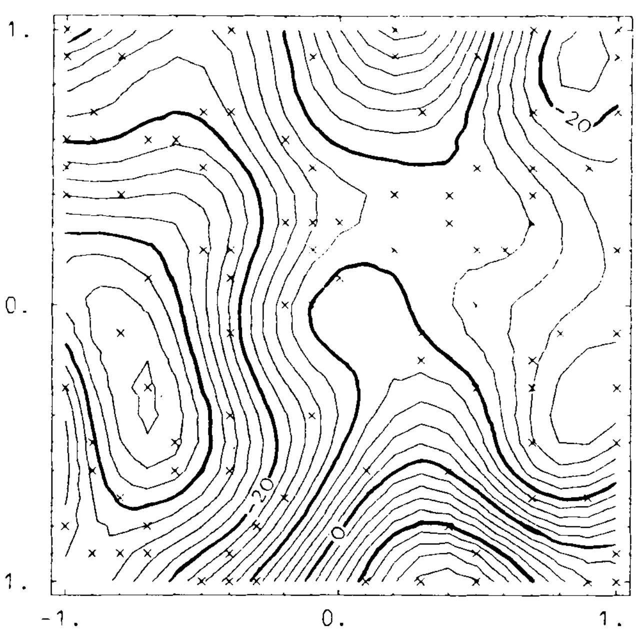

Figure 6. Result of the collocation at sea-level (MCF N). Isoline interval, 2 mGal.

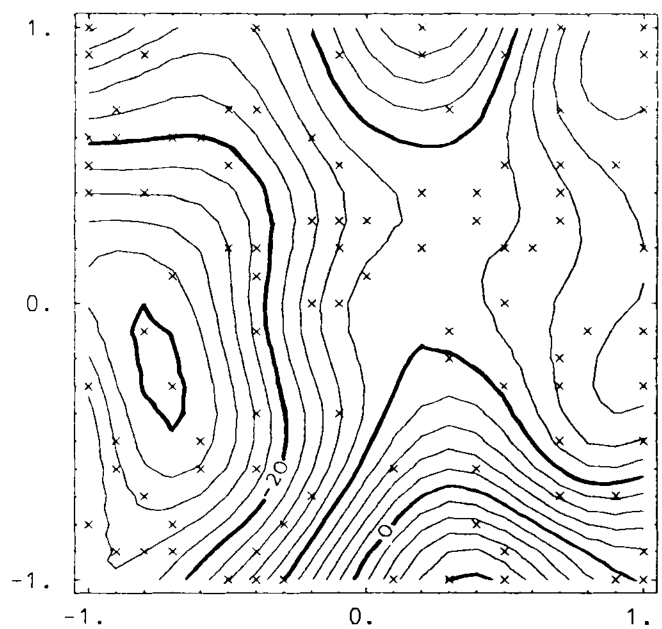

Figure 7. Result of the collocation at 10 km (MCF N) Isoline interval, 2 mGal.

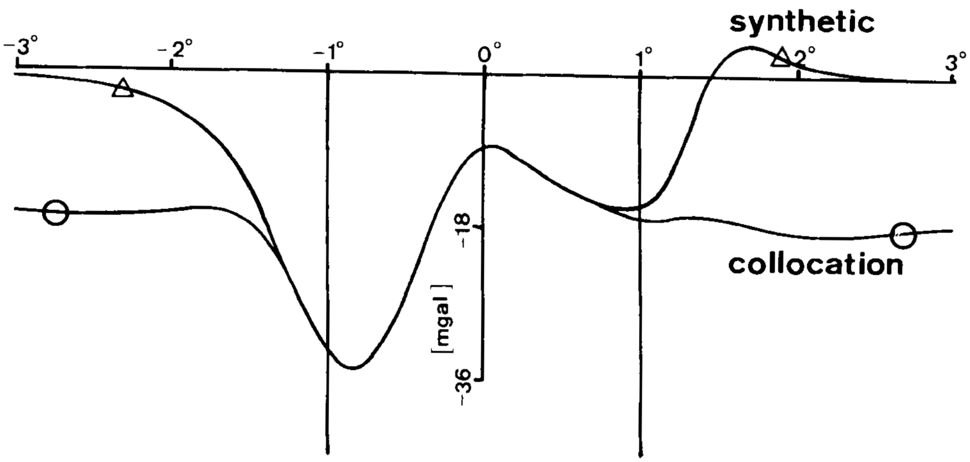

Figure 8. Profile of the synthetic and calculated anomaly at sea-level (at 0° lattitude), ECF N.

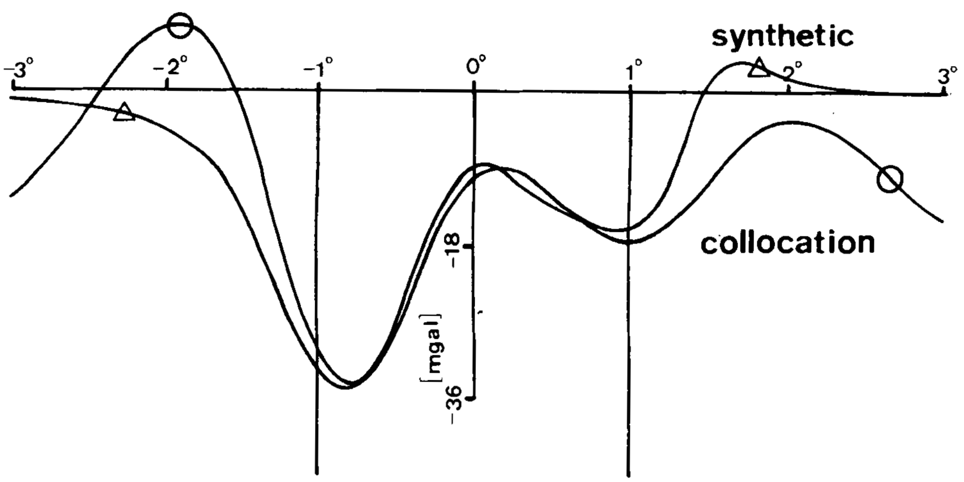

Figure 9. Same as Fig. 8, but ECF L.

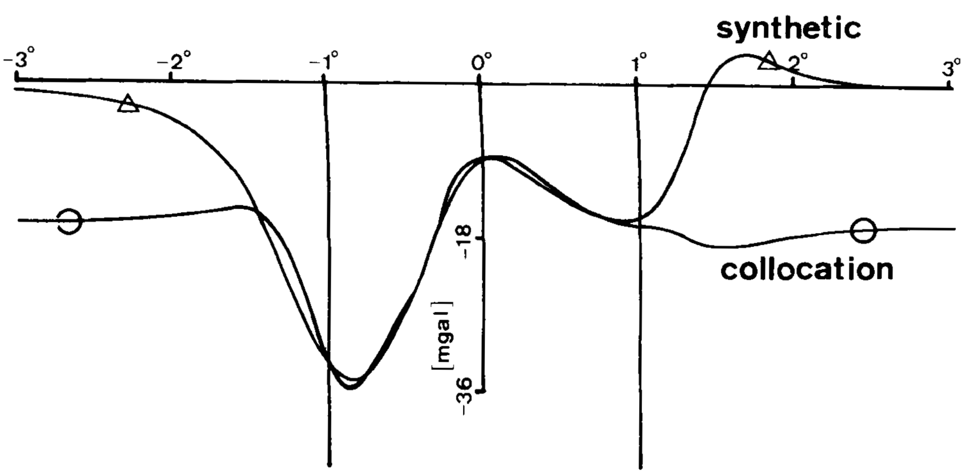

Figure 10. Same as Fig. 8, but ECF S.

Figures 8–10 show profiles at 0° latitude through the gravity field produced by the various MCFs together with the synthetic gravity, both at a height of 0 m.

It becomes apparent that outside the survey area the synthetic gravity converges towards 0 mGal, whilst the gravity field calculated by collocation converges towards the mean value in the survey area.

For MCF L, however, immediate convergence towards this mean value is prevented by the great correlation length. This leads (purely by chance) to a good conformity with the regional gravity field outside the survey area, so that the ensuing mean error $\bar{F}$ for model L remains relatively small. Figs 8 to 10 also clearly show that model N supplies the best conformity within the survey area.

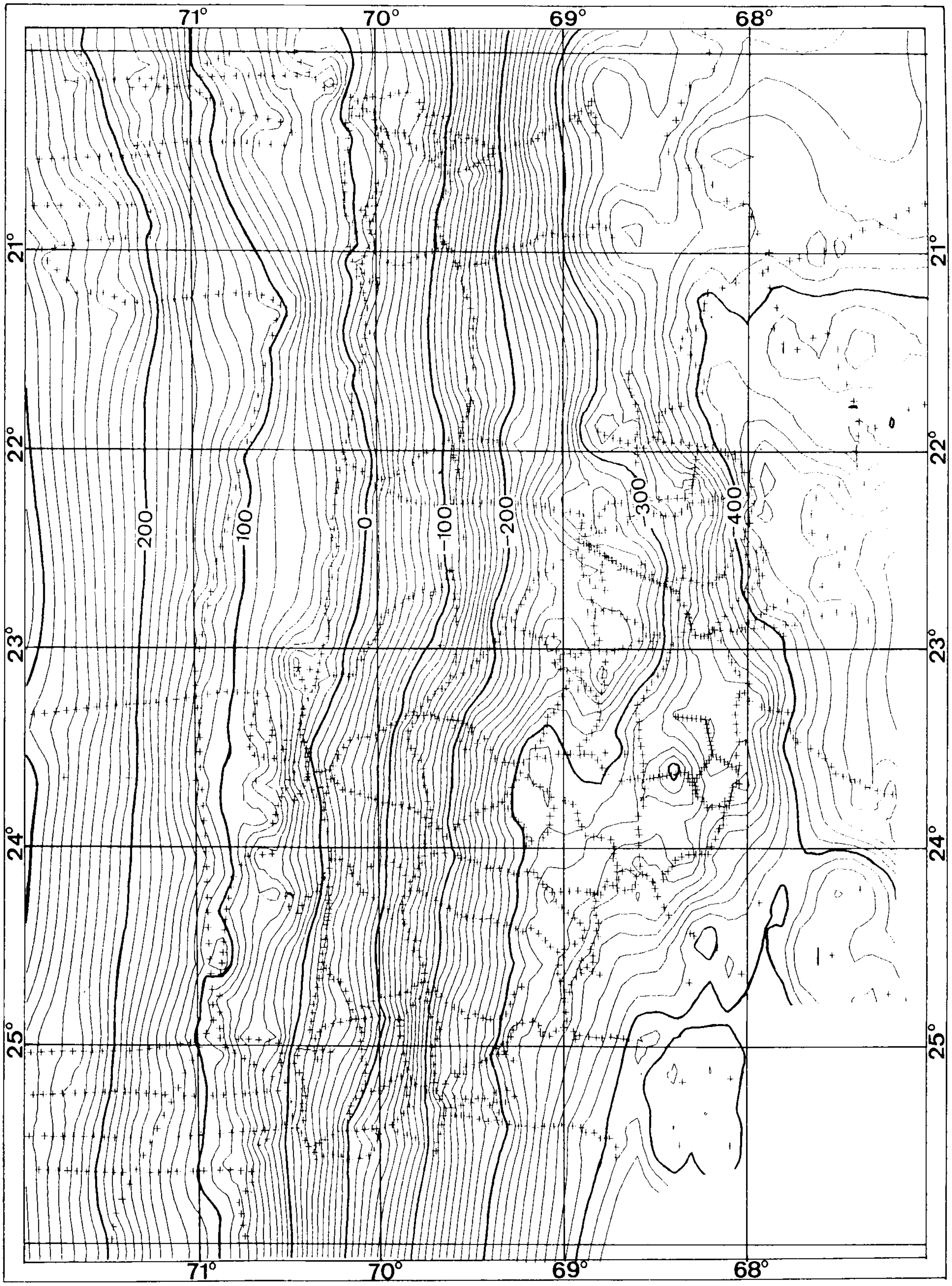

Figure 11. Bouguer anomaly in northern Chile: SCBA. Isoline interval, 10 mGal.

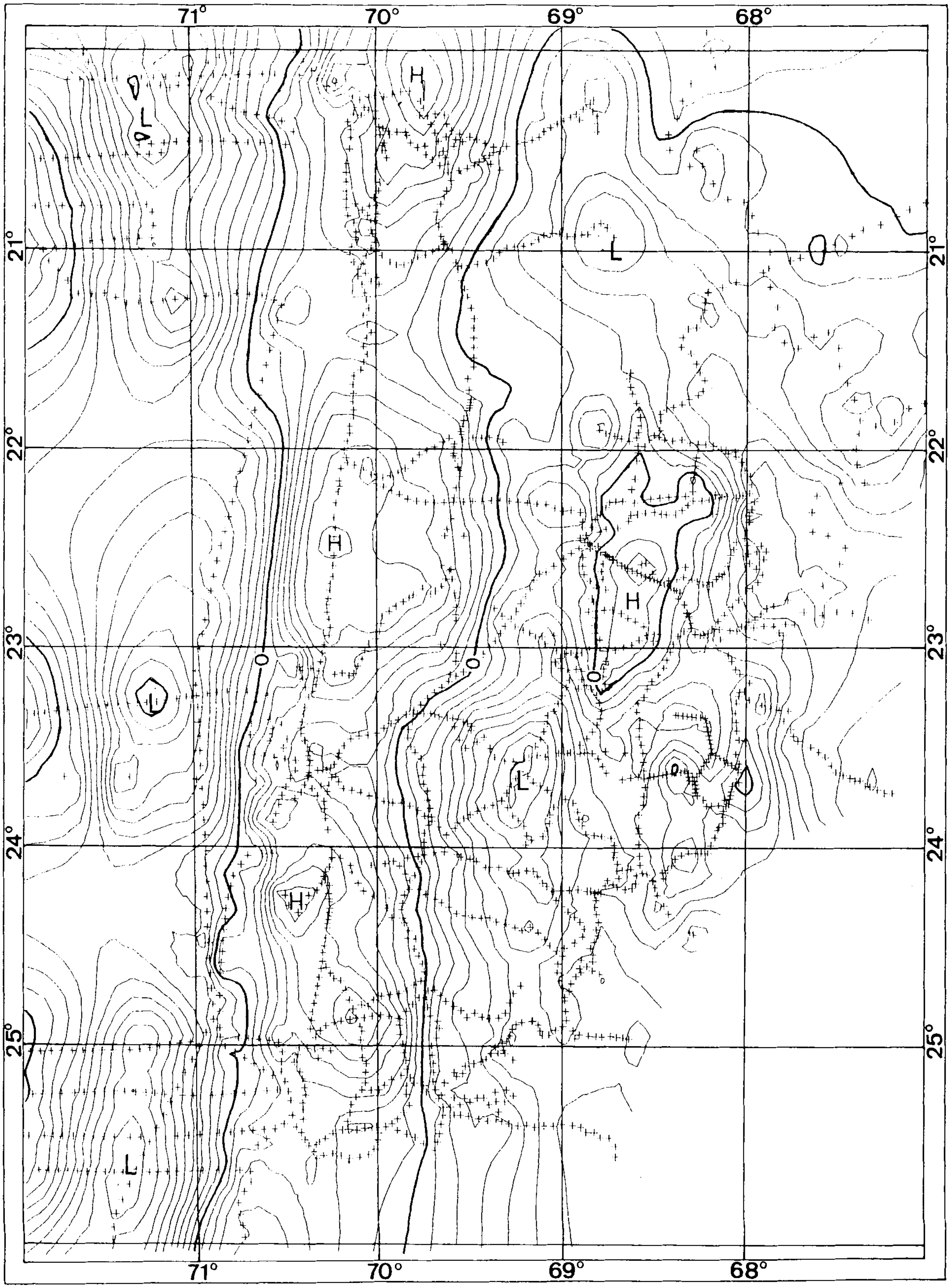

Figure 12. Isostatic anomaly in northern Chile at station level. Isoline interval, 10 mGal.

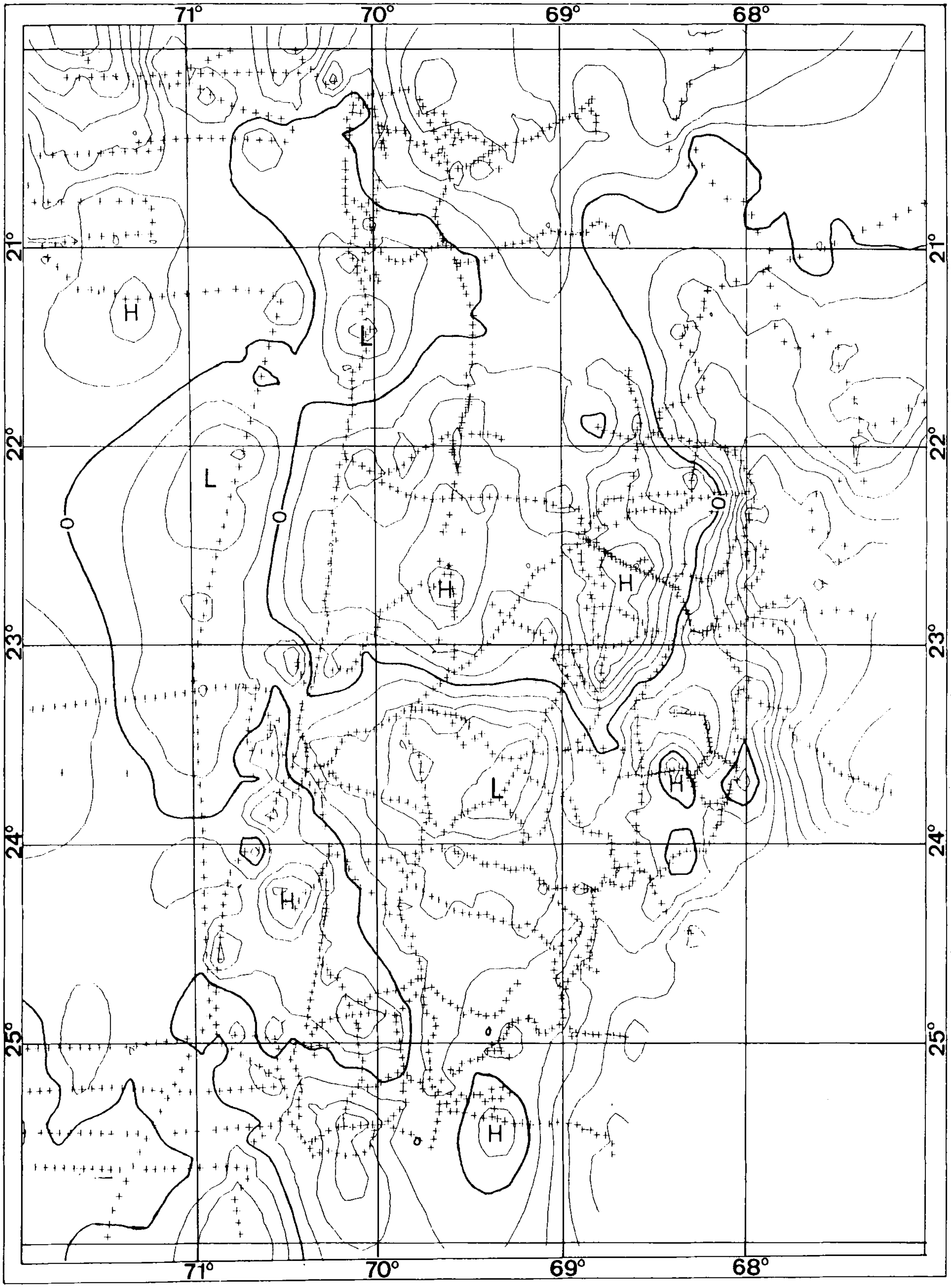

Figure 13. Residual anomaly in northern Chile at station level. Isoline interval, 10 mGal.

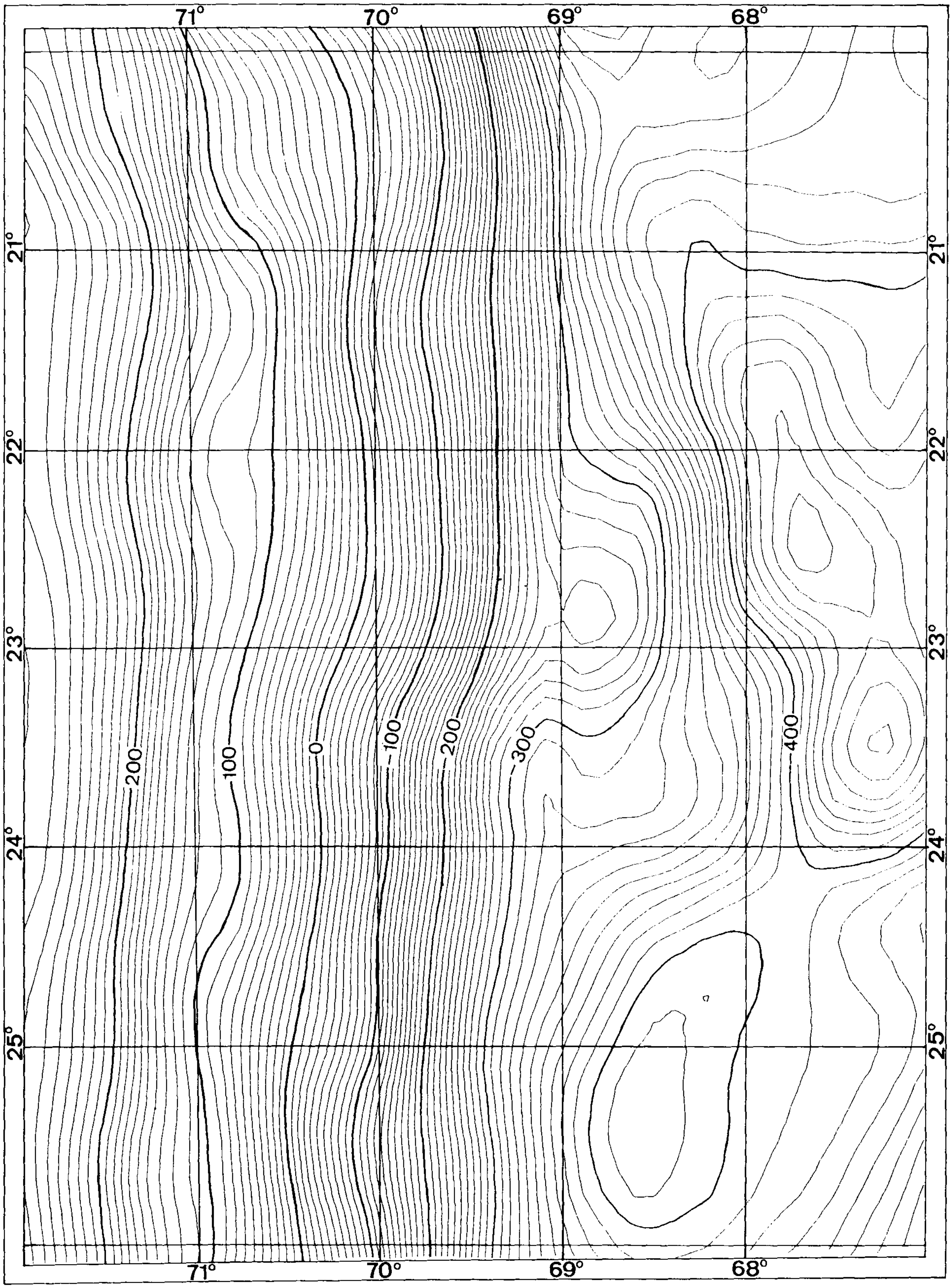

Figure 14. Bouguer anomaly at sea-level: TtCBA, Isoline interval, 10 mGal.

FIELD CONTINUATION OF THE BOUGUER ANOMALY IN NORTHERN CHILE

The Bouguer anomaly (BA) in northern Chile shown in Fig. 11 (Götze *et al.* 1988) was calculated in the normal manner, without consideration for the anomalous vertical gradient, so that as mentioned in the beginning, it is an anomaly at station-level. Special care was taken in the calculation of the topographic reduction. It may be assumed that the Laplace equation is valid between station-level and sea-level. Without this assumption, of course, a field continuation to the sea-level would be impossible. The topographic reduction was carried out up to a distance of about 100 km, using a method developed for gravity investigations in the Alps (Ehrismann *et al.* 1966). Due to the extreme topography (station heights between 0 and 4500 m) and the very irregular station distribution this BA certainly presents a serious problem for any field continuation.

Before the application of collocation simple models were detached from the BA at station-level to reduce the variance of the gravity field which has to be treated with collocation and to make it isotropic. The first model was an isostatic model after Airy with the standard densities.

$$\rho_{\text{crust}} = 2.67\ \text{g/cm}^3$$
$$\rho_{\text{mantle}} = 3.27\ \text{g/cm}^3$$
$$\rho_{\text{water}} = 1.03\ \text{g/cm}^3,$$

and a normal crustal thickness of 40 km, as derived by Giese *et al.* (1983) for the Brasilian craton. This model was calculated directly from the mean heights on a grid $2.5' \times 2.5'$ intended for the topographic reduction, which was completed by $1° \times 1°$ heights at the edges, so that the isostatic reduction could be carried out up to a distance of at least 600 km. For the sake of simplicity point masses were used for the calculation of the effect of the isostatic model. Fig. 12 shows the isostatic anomaly. It has considerably smaller values than the BA; however, it is still very anisotropic due to anomalies running parallel to the trench and which are certainly directly connected to subduction. In order to remove this anisotropy, a model of line masses was built up which are positioned parallel to the trench, with a distance of 0.4° in an east–westerly direction at a depth of 50 km. The size of the line masses was calculated by inversion in such a way that the variance of the remaining residual field became a minimum.

The residual field (Fig. 13) can be considered as almost ideal for the application of collocation due to its isotropy and its minimal variance.

Stable values of $C_0 = 461\ \text{mGal}^2$ and $\psi_{1/2} = 0.55°$ were already obtained after the second step of the iterative procedure for the determination of the MCF. 669 stations were chosen to establish the matrix $\tilde{\mathbf{C}}$ using stepwise collocation.

The assumed error of the measurements of 5 mGal seems at first to be very high. The reason is that small anomalies can not be resolved due to the very irregular distribution of the stations. Similarly, small anomalies produced by erroneous reduction which make downward field continuation impossible can be treated as noise and filtered out. There is no indication of large anomalies also produced by erroneous reduction, as could be caused by a sedimentary basin, for example, so that it may be assumed that downward field continuation is valid.

Figure 14 shows the BA which results for the 0 m level after addition of the two models to the result of collocation. There is a difference of up to 15 mGal for stations above 4000 m in comparison to the normally calculated BA (Fig. 11). This difference is solely caused by the anomalous vertical gradient.

In order to be able to evaluate the increase in accuracy by means of this field continuation the same process was applied to data of a 3-D density model (Strunk 1987) which fits the BA for the same area quite well, locating the model stations at the same position as in reality. The result gave an error of about 8 mGal compared to the synthetic data at 0 m level. Simple interpolation of BA field after Mundry (1970) neglecting the effect of the anomalous vertical gradient led to an error of 24 mGal! It must be noted though that much of this improvement was not achieved by collocation but rather by the models used because these models describe the main part of the BA.

CONCLUSIONS

An application of LSC to a very realistic-looking synthetic gravity anomaly on a topography showed the improvement of carrying out the field continuation from the topography to a reference level compared to simple interpolation, neglecting the effect of the anomalous vertical gradient. Also the predicted error was quite good. The influence of the chosen MCF on the predicted gravity anomaly appeared to be relatively small, whereas the estimated error was admittedly influenced. The application of this technique combined with simple models to data in the Andes of northern Chile and to very similar synthetic data clearly demonstrated that in high mountainous areas the effect of the anomalous vertical gradient cannot be neglected.

Using LSC in the interpretation of gravity data is not limited to the field continuation. All filters which can be applied, e.g. by the FFT method to regularly spaced data become applicable to irregularly spaced data without the need of prior interpolation (Schulz–Ohlberg, personal communication). It is also possible to include in the approximation of the gravity field, e.g. measurements of horizontal components of the gravity field or geoid undulations. However, it has to be pointed out that this is only possible by increasing computational effort, but I think that this is not really a problem in the age of supercomputers.

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