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X-932-76-126

PREPRINT

NASA TM X- 71149

ON ESTIMATING GRAVITY ANOMALIES — A COMPARISON OF LEAST SQUARES COLLOCATION WITH LEAST SQUARES TECHNIQUES

P. ARGENTIERO

B. LOWREY

JUNE 1976

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GREENBELT, MARYLAND

(NASA-TM-X-71149) ON ESTIMATING GRAVITY ANOMALIES: A COMPARISON OF LEAST SQUARES COLLOCATION WITH LEAST SQUARES TECHNIQUES (NASA) 13 p HC $3.50 CSCL 08N

N76-27754

Unclas

G3/46 45873

X-932-76-126
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ABSTRACT

The least squares collocation algorithm for estimating gravity anomalies from geodetic data is shown to be an application of the well known regression equations which provide the mean and covariance of a random vector (gravity anomalies) given a realization of a correlated random vector (geodetic data). It is also shown that the collocation solution for gravity anomalies is equivalent to the conventional least-squares-Stokes' function solution when the conventional solution utilizes properly weighted zero a priori estimates. The mathematical and physical assumptions underlying the least squares collocation estimator are described and its numerical properties are compared with the numerical properties of the conventional least squares estimator.

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INTRODUCTION

The problem of recovering mean gravity anomalies from geodetic data has received much attention. The conventional approach to the problem is to employ the discrete form of Stokes' function to obtain an equation of condition for a least squares estimate of mean gravity anomalies. If the best available a priori estimates of mean gravity anomalies are included with proper weighting in the least squares loss function, the resulting estimates are known to be optimal in a minimum variance sense.[1] This approach has been simulated for satellite perturbation data by Hajela[2], for gradiometer data by Reed[3] and by Argentiero and Garza-Robles[4], and for altimeter data by Gopalapillai[5] and by Argentiero (et al).[6] For insitu data types such as altimetry and gradiometry it can be shown that the procedure can be used to estimate local blocks of anomalies in local blocks of data without significant aliasing.

An alternative approach to geodetic data reduction problems called least squares collocation has been suggested by Moritz.[7] It is claimed that the least squares collocation method is a more general and more powerful parameter estimation procedure than the classical least squares method.[7,8,9,10] It has also been asserted that least squares collocation is the only parameter estimation method which permits the simultaneous and optimal processing of heterogeneous data types.[11,12] Moritz[11] has recommended least squares collocation as the preferred method for estimating mean gravity anomalies from gradiometer data. Rapp[13] and Smith[14] studied the problem of applying the collocation technique to estimating mean gravity anomalies from altimeter data. Rapp[13] asserts that because of the deterministic nature of the Stokes' function, the use of conventional least squares techniques in estimating mean gravity anomalies from altimeter data can lead to false or misleading results. This criticism is repeated by Uotila.[10]

In the following discussion the least squares collocation procedure is viewed as a direct application of the regression equations which provide the conditional mean and covariance of a random vector (mean gravity anomalies) given a realization of a correlated random vector (geodetic data). It will be seen that this approach permits both a fast and simple derivation of the collocation algorithms and a derivation of their precise relationship to the least-squares-Stokes' function algorithm for estimating mean gravity anomalies from geodetic data. Finally the mathematical and physical assumptions underlying the application of the least squares collocation algorithm to the estimation of mean gravity anomalies are discussed.

THE LEAST SQUARES COLLOCATION SOLUTION

In this presentation, least squares collocation will be treated as a parameter estimation procedure in a finite dimensional real vector space. Since for all

practical applications a finite amount of data is processed to estimate a finite number of parameters, no useful generality is lost by this approach.

Let $\{Y'\}$ be a set of geodetic observations. The problem is to obtain from such an observation set a "best" estimate of a set of mean gravity anomalies $\{\delta g\}$. We will define the "best" estimate to be the conditional expectation of $\{\delta g\}$ given a realization of the observations $\{Y'\}$. Since the smallest second moment of a random variable is the second moment about the mean, this is equivalent to applying a minimum variance criterion.

The starting point of the least squares collocation approach to obtaining the best estimate of $\{\delta g\}$ is the assumption that one has full knowledge of the second order statistics of the anomalous potential field everywhere on and outside the reference geoid. (The first order statistics of the anomalous potential field are assumed to be zero.) Let $P(x_1)$ and $P(x_2)$ be the anomalous potentials at points x_1 and x_2 on or outside the reference geoid. We assume the possession of a function $K(x_1, x_2)$ such that

$$E\,(P(x_1)P(x_2)) = K\,(x_1, x_2) \tag{1}$$

The function $K(x_1, x_2)$ is the so-called covariance function, and it is generally defined to be invariant under rotations. Hence the second order statistics of the anomalous potential field are assumed to be independent of location. Let $\{Y\}$ be a vector which is determined by the anomalous potential field and which, after suitable corrections for systematic error sources in the measurement process, is directly observable. Also, let $\{\delta g\}$ be a set of globally distributed gravity anomalies. Since both $\{Y\}$ and $\{\delta g\}$ are determined by the anomalous potential field all second order statistics relating to the two random vectors can be readily derived from the covariance function. Hence define

$$\text{a)}\ E\,(YY^T) = A, \quad \text{b)}\ E\,(\delta g Y^T) = B, \quad \text{c)}\ E\,(\delta g \delta g^T) = C \tag{2}$$

Computational algorithms for obtaining matrices A, B, and C from a covariance function are developed by Moritz[7] and by Tscherning and Rapp.[15] The actual observations $\{Y'\}$ obtained from the instruments are, of course, corrupted by noise. Hence

$$Y' = Y + \nu, \quad E\,(\nu) = \bar{O}, \quad E\,(\nu\nu^T) = Q \tag{3}$$

Equations (2) and (3) permit us to write the joint covariance matrix of the random vectors $\{Y'\}$ and $\{\delta g\}$ as

$$\mathrm{COV}\begin{bmatrix}\delta g\\ Y'\end{bmatrix} = \begin{bmatrix}C & B\\ B^T & A+Q\end{bmatrix} \tag{4}$$

A realization of the random vector $\{Y'\}$ is obtained by means of the actual measurements. Symbolically we do not distinguish between this random vector and its realization. We desire the conditional expectation and the conditional covariance of $\{\delta g\}$ given a realization of the correlated random vector $\{Y'\}$. By assuming either that the random vectors are normally distributed or that the conditional expectation of $\{\delta g\}$ is a linear function of the measurements we can resort to the familiar regression equations for the conditional mean and conditional covariance of a random vector given a realization of a correlated random vector.[1] The results are

$$\delta\hat{g} = B\,(A+Q)^{-1}\,Y' \tag{5}$$

$$\mathrm{COV}\,[\delta\hat{g}] = C - B\,(A+Q)^{-1}\,B^T \tag{6}$$

The solution represented by Equation (5) is the least squares collocation estimate of a global set of gravity anomalies given a covariance function and given the measurement set $\{Y'\}$.

In actuality, one would not attempt to estimate a global set of anomalies from a set of geodetic observations obtained from a certain area. It is only possible to significantly improve knowledge of gravity anomalies in the area covered by the observations. Decompose $\{\delta g\}$ as follows:

$$\delta g = \begin{bmatrix}\delta g_1\\ \delta g_2\end{bmatrix} \tag{7}$$

where $\{\delta g_1\}$ is the set of anomalies covering the region where the measurements are available and where $\{\delta g_2\}$ is the set of anomalies outside of this region. Then the matrix B can be decomposed

$$B = \begin{bmatrix}B_1\\ B_2\end{bmatrix} \tag{8}$$

where

$$B_1 = E\,(\delta g_1 Y^T), \quad B_2 = E\,(\delta g_2 Y^T) \tag{9}$$

The least squares collocation estimate for $\{\delta g_1\}$ becomes

$$\delta\hat{g}_1 = B_1\,(A+Q)^{-1}\,Y' \tag{10}$$

THE CONVENTIONAL LEAST SQUARES SOLUTION EMPLOYING STOKES' FORMULA

The discrete form of Stokes' formula provides a linear relationship between the value of the anomalous potential field at any point and a set of globally distributed mean gravity anomalies. Since $\{Y\}$ is a vector which is determined by the anomalous potential field, Stokes' formula provides a relation between $\{Y\}$ and $\{\delta g\}$ which after suitable linearization can be written as

$$Y = S\ \delta g \tag{11}$$

The elements of the matrix S are obtained by evaluating Stokes' function at the required computation points.

Equation (11) can be used as an equation of condition for a least squares estimate of $\{\delta g\}$. But the resultant solution would not be optimal unless all information were used. Consequently if one accepts the validity of a covariance function it would be proper to utilize the zero vector as an a priori estimate of $\{\delta g\}$ with a weight provided by the inverse of the covariance matrix of Equation (2) c). The resultant loss function to be minimized has the form

$$L\ (\delta\hat{g}) = (Y' - S\ \delta\hat{g})^T Q^{-1} (Y' - S\ \delta\hat{g}) + \delta\hat{g}^T C^{-1}\ \delta\hat{g} \tag{12}$$

The estimator which minimizes the right side of Equation (12) is

$$\delta\hat{g} = (S^T Q^{-1} S + C^{-1})^{-1} S^T Q^{-1} Y' \tag{13}$$

Equation (13) provides the standard least squares solution for $\{\delta g\}$ using Equation (11) as an equation of condition and using the zero vector weighted according to a covariance function as an a priori estimate.

DERIVATION OF AN EQUIVALENCE RELATION

It can be shown that the conventional least squares estimate of $\{\delta g\}$ as defined by Equation (13) and the least squares collocation estimate of $\{\delta g\}$ as defined by Equation (5) are equivalent. Equation (11) defines the zero expectation random vector $\{Y\}$ in terms of the zero expectation random vector $\{\delta g\}$. Thus the covariance matrix of $\{Y\}$ and the joint covariance of $\{Y\}$ and $\{\delta g\}$ can be obtained in terms of the covariance matrix of $\{\delta g\}$. Equation (2) c) provides the covariance matrix of $\{\delta g\}$ as derived from the covariance function of Equation (1). Equation (11) along with Equations (2) c) and (3) permit us to write

$$\mathrm{COV}\begin{bmatrix}\delta g\\ Y'\end{bmatrix} = \begin{bmatrix} C & CS^T \\ SC & SCS^T + Q\end{bmatrix} \tag{14}$$

The regression equation can again be used to obtain the conditional expectation of δg as:

$$\delta\hat{g} = CS^T \ (SCS^T + Q)^{-1} \ Y' \tag{15}$$

A comparison of Equation (4) with Equation (14) yields

$$B = CS^T \ , \quad A = SCS^T \tag{16}$$

Hence the estimate of $\{\delta g\}$ provided by Equation (15) is equivalent to the least squares collocation estimate of Equation (5). We can use the well known Shure matrix identity to translate Equation (15) into the alternative form:

$$\delta\hat{g} = (S^T Q^{-1} S + C^{-1})^{-1} S^T Q^{-1} Y' \tag{17}$$

Equation (17) is identical to Equation (13). This demonstrates that a standard least squares approach to estimating gravity anomalies from geodetic data which utilizes an a priori estimate weighted according to a covariance function yields a solution identical to what is obtained through least squares collocation.

THE DERIVATION OF COVARIANCE FUNCTIONS

The implementation of the collocation technique depends explicitly on the existence of a covariance function which provides the second order statistics of the anomalous potential field. Either of two basic methods may be employed in deriving such a covariance function. Both methods assume that the statistical behavior of the anomalous potential field is independent of location. These methods are summarized below; a detailed exposition may be found in Reference 15.

One method derives the model from a set of ground-based gravitational anomalies, as nearly "global" in scope as is available. The covariance function for mean free air gravity anomalies is estimated as

$$\overline{C}\ (\psi) = \sum \frac{\overline{\delta g}(\phi,\lambda)\,\overline{\delta g}(\phi',\lambda')}{N} \tag{18}$$

where $\overline{\delta g}(\phi,\lambda)$ and $\overline{\delta g}(\phi',\lambda')$ are pairs of mean gravity anomalies in equal area blocks separated by a spherical distance ψ and N is the sum of products at that distance. The covariance function for the anomalous potential can then be obtained as:

$$K(x_1, x_2) = \frac{R^2}{(\ell - 1)^2} \sum_{\ell=0}^{\infty} P_\ell(\cos\psi) \frac{2\ell + 1}{2} \frac{1}{\beta^2 s} \int_0^\pi \overline{C}(\psi') P_\ell(\cos\psi') \sin\psi' \, d\psi' \quad (19)$$

where x_1 and x_2 are two points on or outside the reference geoid which are separated by spherical distance ψ, P_ℓ is the Legendre polynomial function and β and s are in essence geometric factors.

This approach implies that the data set is a random sample of the Earth's gravitational features. In particular, there is an implicit assumption that the characteristics of gravity anomalies over ocean areas are the same as on land, or that the sample contains a proportionate distribution of anomalies over land and ocean areas.

An alternative approach is to obtain the covariance function for the anomalous potential directly from a model for the spherical harmonic coefficients of the potential field. Let $\sigma_\ell^2(\ell)$ be a model for the second moment about zero of normalized spherical harmonic coefficients of degree ℓ. Then the covariance function for the anomalous potential can be written as

$$K(x_1, x_2) = \sum_{\ell=0}^{\infty} s^{\ell+1} (2\ell + 1) \sigma_\ell^2 (\overline{C}_{\ell m}, \overline{S}_{\ell m}) P_\ell \cos(\psi) \quad (20)$$

where again, s is a geometric factor, and ψ is the spherical distance between points x_1 and x_2. One model for the second moment of spherical harmonic coefficients is the well known "Kaula rule of thumb."[16]

$$\sigma_\ell^2 (\overline{C}_{\ell m}, \overline{S}_{\ell m}) = \left(\frac{10^{-5}}{\ell^2}\right)^2 \quad (21)$$

Other models are described in Reference 15.

The implicit assumption of this procedure is that the magnitude of spherical harmonic coefficients decreases monotonically with degree and is representable as a simple function of degree. There are indications that the real field may not have this property.[17] Also the covariance functions derived from the alternative procedures outlined above can differ substantially.[15]

COMMENTS

The least squares collocation algorithms are a form of the regression equations which provide the conditional mean and covariance of a random vector (mean gravity anomalies) given a realization of a correlated random vector (geodetic data). Tapley[18] has shown that the collocation model can be cast into a form in which standard least squares reduction procedures are applicable and that the solution so obtained is identical to the collocation solution. In addition, the conventional approach to estimating mean gravity anomalies from geodetic data which relies on Stokes' formula and a least squares estimation algorithm reduces to the collocation model provided an a priori estimate is weighted according to a covariance function and is included in the loss function. Hence, assertions that the least squares collocation procedure represents a more general and more powerful method for estimating mean gravity anomalies than what is provided by the conventional approach are unfounded.

Several investigators[7,14] have found that the results of a least squares collocation are not sensitive to the choice of a covariance function. The results of this paper provide an explanation of this fact. In effect, the covariance function supplies a weight for a zero a priori estimate of mean gravity anomalies in a least squares reduction procedure. In any meaningful estimation process the resultant solution is dependent mainly on the information content of the data rather than the quality of the a priori estimate. Hence, in a practical simulation or real data reduction one should expect the results of the collocation procedure to be relatively insensitive to the choice of a covariance function. Furthermore, this implies that for most applications the two estimation procedures should yield almost identical results.

If the a priori information provided by a covariance function is to be included in a solution for mean gravity anomalies it is better numerically to do so by means of the Stokes' formula and the conventional least squares method since this procedure involves the inversion of a matrix whose dimension is the number of estimated parameters. The collocation algorithm as given by Equation (10) implies the inversion of a matrix whose dimension is the size of the data set.

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