

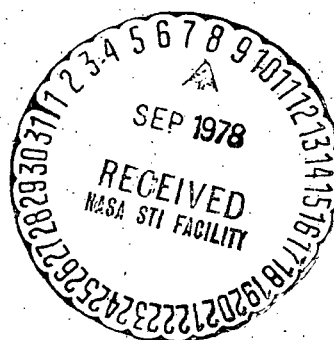


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# On Least Squares Collocation

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### ABSTRACT

It is shown that the least squares collocation approach to estimating geodetic parameters is identical to conventional minimum variance estimation. Hence the least squares collocation estimator can be derived either by minimizing the usual least squares quadratic loss function or by computing a conditional expectation by means of the regression equation.

When a deterministic functional relationship between the data and the parameters to be estimated is available, one can implement a least squares solution using the functional relation to obtain an equation of condition. It is proved the solution so obtained is identical to what is obtained through least squares collocation. The implications of this equivalence for the estimation of mean gravity anomalies are discussed.

# ON LEAST SQUARES COLLOCATION

## INTRODUCTION

A characteristic of geodetic research is that numerous data types are available for estimating parameters of interest. The problems of combining heterogeneous geodetic data types to provide consistent estimates has lead some researchers to the belief that conventional least squares methods are inadequate. An alternative approach to geodetic data reduction problems called least squares collocation has been suggested by Moritz [1]. Some authors have claimed that least squares collocation is a more general and more powerful parameter estimation procedure than the classical least squares method [1, 2, 3, 4, 5]. 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 [6, 7]. Other authors have disputed these claims [8, 9].

This note is an effort to settle what has become a confusing and contentious issue. It will be demonstrated that least squares collocation is an estimator of a type which is well known in conventional estimation theory. The presentation is elementary in content and should be intelligible to anyone familiar with the rudiments of probability theory.

## SOME PROPERTIES OF MINIMUM VARIANCE ESTIMATORS

Let  $X$  be a finite dimensional vector of parameters to be estimated. Since the parameters are not perfectly known it is legitimate to view  $X$  as a random vector. Also there is no loss in generality in assuming the zero vector to be the expectation of  $X$ . Let the covariance matrix of  $X$  be known. Thus:

$$E (XX^T) = C \quad (1)$$

where  $C$  is positive definite. Assume the existence of a finite vector  $Y$  which defines a state which is directly observable. Hence  $Y$  is a random vector which is sampled by a measuring process.

Lacking data, the minimum variance estimate of  $X$  is the zero vector. But intuitively it is clear that if random vectors  $Y$  and  $X$  are correlated and if a realization  $Y'$  of  $Y$  is available, it should be possible to obtain an improved estimate  $\hat{X}$  of  $X$ . Several criteria are available. Two of the most commonly used are

Criterion A – choose  $\hat{X}$  as that vector which minimizes the conventional least squares quadratic form.

Criterion B – choose  $\hat{X}$  as the expectation vector of the conditional distribution of  $X$  given a realization  $Y'$  of  $Y$ .

It will be shown that the application of either criterion leads to the same estimator.

To obtain the improved estimate  $\hat{X}$ , it is necessary to precisely define the correlation between  $Y$  and  $X$ . This is commonly done in two ways which we will describe as a model 1 and model 2. In model 1 the correlation is described by a linear stochastic equation,

$$Y = SX + \nu, E(\nu) = \bar{0}; E(\nu\nu^T) = Q \quad (2)$$

In model 2 the correlation is described in terms of a cross covariance matrix.

$$E \left( \begin{bmatrix} Y \\ X \end{bmatrix} \begin{bmatrix} Y \\ X \end{bmatrix}^T \right) = \begin{bmatrix} A & B \\ B^T & C \end{bmatrix} \quad (3)$$

In fact, models 1 and 2 are alternative and equivalent ways of describing the second order statistical properties of the joint distribution of  $Y$  and  $X$ . Model 1 can be transformed to model 2 by defining the symbols  $A$  and  $B$  on the right side of equation 3 as

$$A = S C S^T + Q \quad B = SC \quad (4)$$

Conversely, model 2 can be converted to model 1 as described in equation 2 with

$$S = BC^{-1} \quad Q = A - BC^{-1}B^T \quad (5)$$

Arbitrarily, we choose model 1 as a description of the necessary correlation. The application of criterion A implies the minimization of the quadratic loss function

$$L(X) = (Y' - SX)^T Q^{-1} (Y' - SX) + X^T C^{-1} X \quad (6)$$

where  $Y'$  is a realization of  $Y$ . The solution to the minimization problem is

$$\hat{X} = (S^T Q^{-1} S + C^{-1})^{-1} (S^T Q^{-1} Y') \quad (7)$$

Equation 7 is known to represent a minimum variance estimator [10].

To apply criterion B, transform model 1 to model 2 by means of equation 4. The well known regression equation [10] can then be employed on the right side of equation 3. The result is

$$\hat{X} = E(X|Y = Y') = B^T A^{-1} Y' \quad (8)$$

Again using equation 4, equation 8 can be transformed into

$$\hat{X} = C S^T (S C S^T + Q)^{-1} Y' \quad (9)$$

The Shure matrix identity can be used to translate equation 9 into the alternative form:

$$\hat{X} = (S^T Q^{-1} S + C^{-1})^{-1} S^T Q^{-1} Y' \quad (10)$$

Equation 10 is identical to equation 7. We have established the following

**Theorem 1** – Assume that  $Y$  and  $X$  are correlated random vectors and that a realization  $Y'$  of  $Y$  is available. The correlation may be defined either in terms

of a linear stochastic equation given by equation 2 or a cross covariance matrix given by equation 3. In each case the minimization of the least squares quadratic loss function of equation 6 and the computation of the expected value of the conditional distribution of  $X$  given  $Y'$  by means of the regression equation yield the same minimum variance estimator.

## LEAST SQUARES COLLOCATION

Let  $Y'$  be a set of geodetic observations. The problem is to obtain from such an observation set an estimate of a set of geodetic parameters  $X$ . The starting point of the least squares collocation approach to the problem is the assumption that one has full knowledge of the second order statistics of the anomalous potential. 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

$$E(P(x_1)P(x_2)) = K(x_1, x_2) \quad (11)$$

Equation 11 defines the so-called covariance function. Let  $\mathcal{L}$  be the countably infinite set of deviations of the spherical harmonic coefficients of the Earth's potential field from reference values. A convenient way to define a covariance function is to specify the second order statistics of  $\mathcal{L}$ . Hence define

$$E(\mathcal{L}\mathcal{L}^T) = T \quad (12)$$

The matrix  $T$  uniquely defines a covariance function. Algorithms for determining the right side of equation 11 given the right side of equation 12 may be found in Moritz [1] or Tscherning and Rapp [11]. Conversely, a given covariance function uniquely defines a covariance matrix  $T$  [12]. Hence there is no loss in generality in assuming that the covariance function for the least squares collocation procedure is given in terms of a matrix  $T$  as defined by equation 12. Let  $Y$  be the ideal observation state of which  $Y'$  is a realization. Since both  $Y$  and  $X$  are geodetic entities they are functions of the set of spherical harmonic coefficients of the Earth's potential. First order Taylor series expansions of these functions about a set of reference spherical harmonics will yield linear matrix equations

$$\begin{aligned} \text{a, } Y &= f_1 \mathcal{L} \\ \text{b, } X &= f_2 \mathcal{L} \end{aligned} \quad (13)$$

where reference values of  $Y$  and  $X$  are assumed equal to the zero vector. In equations 13 and in subsequent equations, whenever the matrix symbolism implies countable infinite summation it is the limiting value which is intended. Alternatively, the reader can assume that the

vector  $\mathcal{L}$  of deviations of spherical harmonic coefficients from reference values is truncated at a sufficiently high degree that errors in representation in equations 13 are negligible.

Equations 12 and 13 yield

$$\begin{aligned} \text{a, } E(Y Y^T) &= A = f_1 T f_1^T \\ \text{b, } E(X X^T) &= C = f_2 T f_2^T \\ \text{c, } E(Y X^T) &= B = f_1 T f_2^T \end{aligned} \quad (14)$$

The actual observations  $Y'$  are corrupted by errors in the measuring system. Hence

$$Y' = G Z + Y + \nu \quad (15)$$

where

$$\begin{aligned} \text{a, } E(\nu) &= \bar{0}, \\ \text{b, } E(\nu \nu^T) &= Q, \\ \text{c, } E(z) &= \bar{0}, \\ \text{d, } E(z z^T) &= P, \end{aligned} \quad (16)$$

The vector  $Z$  is interpreted as a set of parameters which determines the systematic part of the errors in the measuring system. Define an augmented parameter set as

$$S = \begin{bmatrix} X \\ Z \end{bmatrix} \quad (17)$$

Equations 14, 15 and 16 define the correlation between random vectors  $Y'$  and  $S$ . In the previous section it was demonstrated that given the correlation between two random vectors and given a realization of one of the vectors, it was possible to construct a minimum variance estimator for the other vector. This estimator can be obtained either by using the regression equation to compute a conditional mean or by minimizing a conventional least squares quadratic loss function. Arbitrarily we will obtain the minimum variance estimate for  $S$  by computing the conditional mean of  $S$  given a realization of  $Y'$ . The covariance matrix for the joint distribution of  $S$  and  $Y'$  is

$$E\left(\begin{bmatrix} Y' \\ S \end{bmatrix} \begin{bmatrix} Y' \\ S \end{bmatrix}^T\right) = \begin{bmatrix} A + G P G^T + Q & F \\ F^T & D \end{bmatrix} \quad (18)$$

where

$$\begin{aligned} \text{a, } F &= [B, GP] \\ \text{b, } D &= \begin{bmatrix} C & 0 \\ 0 & P \end{bmatrix} \end{aligned} \quad (19)$$

Let  $S_c$  be the conditional distribution of  $S$  given a realization of  $Y'$ . By assuming either that the random vectors are normally distributed or that the expectation of  $S_c$  is a linear function of the measurements, we can resort to the regression equations for the mean and covariance of  $S_c$  as

$$E(S_c) = \hat{S} = F^T (A + G P G^T + Q)^{-1} Y' \quad (20)$$

$$E\left((S_c - \hat{S})(S_c - \hat{S})^T\right) = D - F^T (A + G P G^T + Q)^{-1} F \quad (21)$$

Equations 17, 19, and 20 permit us to separately write the conditional expectations of  $X$  and  $Z$  as

$$\begin{aligned} \text{a, } \hat{X} &= B^T (A + G P G^T + Q)^{-1} Y' \\ \text{b, } \hat{Z} &= P G^T (A + G P G^T + Q)^{-1} Y' \end{aligned} \quad (22)$$

A straightforward application of the Shure matrix identity converts equations 22 into

$$\begin{aligned} \text{a, } \hat{X} &= B^T (A + Q)^{-1} (Y' - G \hat{Z}) \\ \text{b, } \hat{Z} &= (G(A + Q)^{-1} G^T + P^{-1})^{-1} G^T (A + Q)^{-1} Y' \end{aligned} \quad (23)$$

Equations 23 represent the least squares collocation solution for geodetic parameters  $X$  and measuring system parameters  $Z$  given a realization of observation vector  $Y'$ . We have proved the following.

**Theorem 2:** The least squares collocation solution for geodetic parameters  $X$  and measuring system parameters  $Z$  given a realization of an observation vector  $Y'$  is

identical to the conventional minimum variance solution. Hence the collocation solution can be obtained either by determining the conditional expectations of  $X$  and  $Z$  by means of the regression equation or by minimizing the usual least squares quadratic loss function.

Tapley [8] provides a somewhat longer proof of the equivalence of least squares collocation to the conventional minimum variance estimator. Tapley's proof is interesting because it relies entirely on elementary matrix operations.

## APPLICATIONS

The previous sections show that the techniques of conventional minimum variance estimation have considerable power and generality. With the appropriate use of these techniques, one can obtain a minimum variance estimate of any set of parameters which are functions of the anomalous potential given a realization of any observation set which is also a function of the anomalous potential. In many cases it is possible to augment the parameter set in question in such a way that the laws of Mathematical Geodesy provide a deterministic functional relationship between the augmented parameter set and the ideal or noiseless representation of the data set. For this situation two different estimation procedures are available:

Estimation Procedure 1) Use the postulated covariance matrix for the anomalous spherical harmonic coefficients to construct the covariance matrix for the joint distribution of the data set and the parameter set to be estimated. The regression equation can then be used to compute the conditional mean of the parameter set. (least squares collocation)

Estimation Procedure 2) Use the postulated functional relationship between the augmented parameter set and the data set to construct an equation of condition for a conventional least squares with a priori estimation of the parameter set.

It will be shown that the two procedures are equivalent. Again let  $T$  represent the covariance matrix for the anomalous spherical harmonic coefficients  $\mathcal{L}$ . Let  $Y$  be the ideal or noiseless representation of the data and let  $X_1$  be the parameter set to be estimated. Assume that  $X_1$  is part of a larger parameter set. Hence

$$S = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \quad (24)$$

The vectors  $Y$  and  $S$  are functions of the anomalous potential. First order Taylor series expansions of the appropriate functions yield linear matrix equations

$$\begin{aligned}
&\text{a, } Y = f_1 \mathcal{L} \\
&\text{b, } X_1 = f_{2,1} \mathcal{L} \\
&\text{c, } X_2 = f_{2,2} \mathcal{L}
\end{aligned} \tag{25}$$

Equations 25b and 25c can be rewritten as

$$S = f_2 \mathcal{L} \tag{26}$$

where

$$f_2 = \begin{bmatrix} f_{2,1} \\ f_{2,2} \end{bmatrix} \tag{27}$$

For simplicity assume that there are no systematic errors in the measuring system. Then the observation equation is

$$Y' = Y + \nu, E(\nu) = \bar{0}, E(\nu\nu^T) = Q \tag{28}$$

Equations 25 and 28 permit us to write

$$\begin{aligned}
&\text{a, } E(Y' Y'^T) = f_1 T f_1^T + Q \\
&\text{b, } E(Y' X_1^T) = f_1 T f_{2,1}^T
\end{aligned} \tag{29}$$

The least squares collocation solution for  $X_1$  is

$$\hat{X}_1 = f_{2,1} T f_1^T (f_1 T f_1^T + Q)^{-1} Y' \tag{30}$$

To implement estimation procedure 2, assume that the laws of Mathematical Geodesy provide a deterministic functional relationship between  $Y$  and  $S$ . A first order Taylor series expansion of the function will yield

$$Y = f_3 S \tag{31}$$

Notice that from equations 25a, 26 and 31 we have

$$f_1 = f_3 f_2 \tag{32}$$

Given equations 28 and 31, the usual least squares solution for S is given by

$$\hat{S} = \left( f_3 Q^{-1} f_3^T + (f_2 T f_2^T)^{-1} \right)^{-1} f_3^T Q^{-1} Y' \quad (33)$$

Transform equation 33 to the equivalent form

$$\hat{S} = f_2 T f_2^T f_3^T (f_3 f_2 T f_2^T f_3^T + Q)^{-1} Y' \quad (34)$$

With the aid of equation 32, equation 34 can be rewritten as

$$\hat{S} = f_2 T f_1^T (f_1 T f_1^T + Q)^{-1} Y' \quad (35)$$

Hence

$$\hat{X}_1 = f_{2,1} T f_1^T (f_1 T f_1^T + Q)^{-1} Y' \quad (36)$$

Equation 36 is identical to equation 30 and this proves the equivalence.

The results of this section have important consequences for the estimation of mean gravity anomalies. Stokes' formula provides a representation of the anomalous potential on or outside of a reference geoid as [13]

$$U(r, \phi, \lambda) = \frac{R}{4\pi} \iint_{\sigma} S(r, \psi) \delta g \, d\sigma \quad (37)$$

where  $r$ ,  $\phi$ , and  $\lambda$  are the spherical coordinates of the computation point,  $R$  is the value of the Earth's radius,  $S(r, \psi)$  is the Stokes function with  $\psi$  the spherical distance between the integration point and the projection of the computation point on the reference geoid. The symbol  $\delta g$  is the point gravity anomaly referenced to the nominal field and measured on the reference geoid. The integration is over the entire geoid. The discrete approximation to Stokes' formula is

$$U(r, \phi, \lambda) = \frac{R}{4\pi} \sum_i S(r, \psi_i) \overline{\delta g_i} \, d\sigma_i \quad (38)$$

where  $\overline{\delta g_i}$  is interpreted as a mean gravity anomaly averaged over a non-zero surface area  $d\sigma_i$ . The summation of equation 38 is finite and encompasses the entire reference geoid. Let  $Y$  be a vector which is determined by the anomalous potential field. Assuming the

validity of the discrete form of Stokes' formula, equation 38 provides a relationship between  $Y$  and a globally distributed set  $\overline{\delta g}$  of mean gravity anomalies which after suitable linearization can be written as

$$Y = f \overline{\delta g} \quad (39)$$

Equation 39 can be used as an equation of condition for a least squares with a priori estimate of a global set of mean gravity anomalies. On any subset of the globally distributed mean gravity anomalies the solution so obtained will agree with the least squares collocation solution.

## COMMENTS

The least squares collocation algorithm can be exhibited as a conventional minimum variance estimator. Hence, the algorithm can be derived either as an application of the regression equation or by minimizing the usual least squares quadratic form. In some cases a geodetic parameter set to be estimated can be augmented in such a way that the laws of Mathematical Geodesy provide a deterministic relation between the augmented parameter set and the available data. For this case the deterministic relation can be used to obtain an equation of condition for a conventional least squares with a priori estimate. The solution so obtained must agree with the least squares collocation solution.

For estimating mean gravity anomalies, both least squares collocation and the conventional least squares approach utilizing Stokes' formula are applicable. Each procedure must employ a certain approximation. With the conventional least squares approach an integral representation (equation 37) is replaced by a finite sum (equation 38). With least squares collocation, covariance and cross covariance representations for point gravity anomalies must be averaged to obtain similar representations for mean gravity anomalies. In each case the approximations can be performed so that the errors of representation are less than any preassigned value. The results of this paper show that if the two estimation procedures are implemented in such a way that corresponding errors of representation are negligible, resulting estimates of mean gravity anomalies will be equal. Hence, the choice between estimation procedures should be made on the basis of computational convenience.

A disadvantage of the conventional least squares approach to estimating mean gravity anomalies which relies on a discrete form of Stokes' formula is that its rigorous implementation implies the simultaneous estimation of a global set of anomalies. With the least squares collocation approach it is convenient to estimate anomalies on a one by one basis. However, it can be shown that for many data types and with proper estimation strategies [14, 15, 16, 17], it is possible to estimate local blocks of mean gravity anomalies without serious aliasing.

A serious computational problem associated with least squares collocation is that its implementation implies the inversion of a matrix whose dimension is the size of the data

set. The conventional least squares approach implies the inversion of a matrix whose dimension is the size of the parameter set to be estimated. Hence, when large and dense data distributions are available for estimating mean gravity anomalies a conventional least squares technique utilizing Stokes' formula is a more logical choice for an estimation procedure.

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