

COLLOCATION AND LEAST SQUARES METHODS AS A TOOL FOR HANDLING
GRAVITY FIELD DEPENDENT DATA OBTAINED THROUGH SPACE RESEARCH TECHNIQUES

C.C. Tscherning

Geodætisk Institut
Gamlehavn Allé 22
DK-2920 Charlottenlund, Danmark

ABSTRACT

Least squares adjustment and collocation methods have in the last decade been the tool for extracting gravity field information from data obtained through space research techniques (satellite orbit tracking, altimeter observations, doppler determined positions), and when combining these data with data observed at the surface of the Earth.

The mathematical framework for the two models is described and the models are compared. It is shown that the two methods only become equivalent in cases where the number of parameters are equal to the number of observations.

It is pointed out that several arbitrary choices (of parameters, weights and norms) will have to be made before the methods can be applied, and that further investigations are needed in order to justify the specific choices.

Keywords: Geodesy, gravity field, collocation, least squares adjustment, mathematical model

1. INTRODUCTION

A knowledge of the gravity potential of the Earth is required in order to solve problems in navigation, geodesy, oceanography and solid earth physics (see Refs. 29-32, 18). And a special branch of geodesy, physical geodesy, has as its main task the determination of the gravity potential.

Earlier it was envisaged that the gravity potential could be determined as a solution to a certain boundary value problem for the Laplace operator. The boundary values were the gravity anomalies, for which a global coverage were required.

But also other quantities give information about the gravity potential, namely astronomical latitude and longitude (which give the direction of the gravity vector) and the gravity gradients. Further types of quantities became available by the advent of the artificial satellites. These quantities were (and is) obtained by satellite tracking or by remote sensing techniques. Satellites equipped with gradiometers will make further types of observations available. Finally we should not forget, that geopotential heights, obtained by levelling, in combination with cartesian coordinates (determined e.g. by doppler techniques) in itself is informa-

tion about the gravity potential.

It is the purpose of this paper to discuss two currently applied methods for the handling of this heterogeneous dataset. In Section 2 we describe the basic characteristics of the mathematical framework within which the gravity potential can be considered. We discuss in Section 3 least squares adjustment methods, in Section 4 the least norm collocation method and in Section 5 the least squares collocation method. This method is a collocation method where the norm has been selected so that a least square condition is fulfilled. Finally in Section 6 we describe some of the applications of the methods and discuss some of the problems associated with these applications.

2. THE MATHEMATICAL MODEL FOR THE GRAVITY FIELD

The gravity potential, W , is the sum of the gravitational potential, V , and the rotational potential. Let us suppose that we have adopted a certain reference potential, U , which rotational part is equal to that of W and which contains the influence of all masses outside the surface of the Earth (the atmosphere, the moon, the sun, etc.). Then $T = W - U$ is called the anomalous potential and it is a harmonic function outside the surface of the Earth. Let us denote the set of harmonicity by Ω . Points in Ω (or in \mathbb{R}^3) will be denoted P, Q , with spherical coordinates (φ, λ, r) , (φ', λ', r') , respectively. (φ = geocentric latitude, λ = longitude and r = distance from the origin).

The anomalous potential will be an element of a linear vector space of functions harmonic in Ω , $H(\Omega)$. The vector space may be equipped with inner products, (\cdot, \cdot) , which will have a corresponding norm, $\|\cdot\|$. (We will distinguish between different inner products or norms by a subscript.) The elements of $H(\Omega)$ for which a norm is finite will form a so-called Hilbert space. The spaces will be infinite dimensional, but separable, i.e. a countable basis exists. (We have to put some small restrictions on Ω and not all norms will do).

The anomalous potential will be an element of such a space, for example with norm given by

$$\|T\|_0^2 = \frac{1}{4\pi} \int_{\Omega} T(P)^2 d\Omega \quad (1a)$$

or

$$\|T\|_1^2 = \frac{1}{4\pi} \int_{\Omega} (T(P)^2 + (\nabla T)^2) d\Omega, \quad (1b)$$

where ∇T is the gradient of T .

In Hilbert spaces any element may be represented by its expansion with respect to a complete, orthonormal system. Had Ω been the set outside a sphere with radius R we would have

$$T(P) = \frac{GM}{r} \sum_{i=0}^{\infty} \left(\frac{R}{r}\right)^i \sum_{j=0}^i \bar{P}_{ij}(\sin\varphi) [\bar{C}_{ij} \cos j\lambda + \bar{S}_{ij} \sin j\lambda], \quad (2)$$

where GM is equal to the product of the gravitational constant and the mass of the Earth, \bar{P}_{ij} are the fully normalized associated Legendre polynomials and \bar{C}_{ij} , \bar{S}_{ij} are the coefficients of the series. The orthonormal base is, using $\|\cdot\|_0$ or $\|\cdot\|_1$, given by (1a,b), formed by the functions

$$k_{ij} \frac{1}{r} \left(\frac{R}{r}\right)^i \bar{P}_{ij}(\sin\varphi) \begin{cases} \cos j\lambda \\ \sin j\lambda \end{cases} \quad (3)$$

where k_{ij} is a normalization factor.

The set of solid spherical harmonics (3) will be a complete (but not generally orthonormal) base in all so-called regular Hilbert spaces, which are subspaces of $H(\Omega)$. The anomalous potential may therefore be approximated arbitrarily well by a finite linear combination of these solid spherical harmonics, i.e. for all $\epsilon > 0$ there exist an integer N , and a set of constants C'_{ij} , S'_{ij} , so that

$$\|T(P) - \sum_{i=0}^N \frac{GM}{r} \left(\frac{R}{r}\right)^i \sum_{j=0}^i \bar{P}_{ij}(\sin\varphi) \{ C'_{ij} \cos j\lambda + S'_{ij} \sin j\lambda \} \| < \epsilon. \quad (4)$$

The set of functions (3) are not the only set of "reasonable" functions which form a complete basis, and which therefore may be useful when determining approximations to T . Other sets are potentials produced by point masses, surface layers or Stokes function with one point held fixed. The quantities corresponding to the "potential coefficients" will then be the values of a set of point masses, surface densities or gravity anomalies, respectively. (Such bases have been considered e.g. in (Refs. 2, 3, 21, 1)).

Corresponding to a Hilbert space, H , there exist another Hilbert space called the dual space, H^* . This space consist of the continuous linear functionals which are mappings from H to the real numbers. These linear functionals are extremely important because an observed quantity generally is or will have to be expressed as the value of a linear

functional applied on an element of the Hilbert space. A point gravity anomaly is for example equal to

$$\left(-\frac{\partial}{\partial r} \Big|_P - \frac{2}{r} \text{ev}_P\right)T = -\frac{\partial T}{\partial r} - \frac{2}{r} T(P) = \Delta g,$$

where ev_P is the evaluation functional in the point P , and T may be considered an element of a Hilbert space with the norm $\|\cdot\|_0$, cf. eq. (1a).

A wide range of Hilbert spaces of harmonic functions will have a reproducing kernel. Such a kernel, $K(P,Q)$ is a mapping from $\Omega \times \Omega$ to the real numbers. It will, for either P or Q fixed, be an element of the Hilbert space and it will have the reproducing property

$$(K(P,Q), T(P)) = T(Q), \quad Q \in \Omega, \quad (5)$$

This kernel may for Ω being the set outside a sphere and for certain types of inner products be computed explicitly by closed expressions. It is the existence of this reproducing kernel which makes it possible to apply the method of collocation in practice, cf. Section 4.

This above described functional analytic model has a statistical counterpart. Here the anomalous potential is related to a stochastic or random process. The process may be formed by a basic set of stochastic or random variables $X_P: H(\Omega) \rightarrow R$, which as outcome has the value of a harmonic function in a point, P . A linear vector space may be formed by taking the set of all finite linear combinations of these random variables. This space is equipped with an inner product, namely defined as being equal to the covariance of two random variables. This space may be completed and (the dual to) a Hilbert space with reproducing kernel is formed, the reproducing kernel being equal to the covariance function of the basic random variables, $\text{cov}(X_P, X_Q) = K(P,Q)$.

The basic for forming this stochastic process is the adoption of a joint probability distribution for the random variables. This distribution will have to be prescribed e.g. by supposing the random variables to be Gaussian distributed with mean value zero and covariance given through a positive definite function of $\Omega \times \Omega \rightarrow R$. This function must be harmonic in each of its variables, because the elements of the sample space are harmonic functions. It is not possible to estimate the probabilistic properties, because we have no possibility for repeating our observations at another Earth. See (Ref. 26) for a clarification of this point.

Further details about the functional analytic and the stochastic model can be found in (Refs. 25, 33, 34, 26, 13, 9, 77).

3. LEAST SQUARES ADJUSTMENT

It is (to a good approximation) possible to express the relationship between T and observed quantities (which only depend on T) in the form of linear functionals (L_i) applied on T ,

$$L_i(T) + n_i = m_i, \quad (6)$$

where m_i is the measured quantity, $L_i(T)$ is the "true" quantity and n_i is the measurement error, (noise). In case we suppose that the measurements only depend on e.g. the low order potential coefficients or a finite set of mean surface density values eq. (6) may be written

$$\sum_{j=1}^N B_{ij} s_j + n_i = m_i \quad (7)$$

Here s_j , $j=1, \dots, N$ are potential coefficients or density values.

In case the observed quantities also depend on other parameters (e.g. tracking station coordinates or transformation parameters) we have

$$\sum_{k=1}^M A_{ik} X_k + \sum_{j=1}^N B_{ij} s_j + n_i = m_i \quad (8)$$

(Note, that even if a specific kind of parameters have been selected, the parameters are not necessarily unique (potential coefficients may be normalized in different ways)).

Having an apriori knowledge of the statistical characteristics of the noise, the eq. (8) is what is required for a least squares adjustment, presupposed the number of observations exceeds the number of parameters $N + M$. The least squares condition to be fulfilled is

$$\{n_i\}^T \{P_{ij}\}^{-1} \{n_j\} = \min \quad (9)$$

where $\{P_{ij}\}$ is the variance-covariance matrix of the noise or error quantities.

As a result of the adjustment, parameters \bar{s}_j are obtained, and we have thereby got a estimate \tilde{T} of the anomalous potential,

$$\tilde{T}(P) = \sum_{j=1}^N \bar{s}_j V_j(P), \quad (10)$$

where V_j , $j=1, \dots, N$ generally are harmonic functions (solid spherical harmonics, potentials of unit point masses or surface densities, spline functions or similar functions).

It is well-known from approximation theory, that an estimated function may happen to oscillate very much in between data-points. A remedy against this is the requirement that the (weighted) squaresum of the parameters plus the left hand side of eq. (9) becomes a minimum,

$$\sum_{i=1}^N p_i s_i^2 + \sum_{k=1}^M q_k X_k^2 + \{n_i\}^T \{P_{ij}\}^{-1} \{n_j\} = \min. \quad (11)$$

A solution to this minimum problem can be found in (Refs. 68,81). Note, that instead of weights p_i and q_i , weight-matrices could have been used

and that we now also may consider "underdetermined" adjustment problems, i.e. $N+M$ greater than or equal to the number of observations.

The quantities $\sum_{i=1}^N p_i s_i^2$ and $\sum_{k=1}^M q_k X_k^2$ are

examples of norms in a finite (N) dimensional space of harmonic functions and a finite (M) dimensional space of real numbers. The application of eq. (11) in an adjustment procedure should therefore be denoted a combined least squares and minimum norm adjustment.

It is worth noting, that adjustment procedures are not limited to "global" problems. In many cases it is possible to find a linear independent set of harmonic functions well suited for representing local information. Such a set may be potentials generated by unit point masses situated near the surface of the Earth, potentials generated by surface density layers or, as we shall see in Section 4, harmonic functions obtained by applying a linear functional on a reproducing kernel.

4. COLLOCATION

Let us to a start suppose that our observed quantities may be expressed as linear functionals L_i applied on T and that they have no errors,

$$L_i(T) = m_i \quad (12)$$

Methods for the determination of an approximation \tilde{T} to T which agrees with the observations, i.e.

$$L_i(\tilde{T}) = m_i \quad (13)$$

are denoted collocation methods. It is natural to require that \tilde{T} has some of the same properties as have T , namely that it is harmonic in Ω and that it has the same degree of smoothness as T . This can be expressed by requiring \tilde{T} to be an element of a Hilbert space (H) of harmonic functions. When this space has a reproducing kernel $K(P, Q)$ and the functionals L_i are elements of the dual space H^* , a unique solution to the approximation problem may be constructed. The uniqueness is obtained by requiring \tilde{T} to have the minimum norm in between all elements of H which fulfil eq. (13). The approximation is given by

$$\tilde{T}(P) = \sum_{i=1}^M a_i L_i K(P, \cdot) \quad (14)$$

where the constants a_i are determined by

$$\{L_i L_j K(\cdot, \cdot)\} \cdot \{a_i\} = \{m_j\} \quad (15)$$

A condition for solution is that the matrix $\{L_i L_j K(\cdot, \cdot)\}$ is regular, or equivalently that the linear functionals are linear independent.

When the dimension of H is finite, N, equal to the number of observation, a solution to the collocation

tion problem may be found simply by solving a set of linear equations

$$\{L_i(f_j)\} \{a_j\} = \{m_i\}$$

where then

$$\tilde{T}(P) = \sum_{i=1}^N a_i f_i.$$

The set f_i must be a basis for H . For a special selection of data points and functions f_i the matrix $\{L_i(f_j)\}$ becomes the unit matrix, and we have the sampling function approach of (Ref. 11). It is well known, that the approximation $\tilde{T}(P)$ will depend strongly on the dimension, N .

Let us again regard the situation where a unique solution is obtained due to the condition of minimum norm. Here absolute error bounds may be computed for \tilde{T} when $T \in H$ and $\|T\|$ is known. For the numerical difference between the true value $L(T)$ and the computed value $L(\tilde{T})$ an inequality will hold (cf. Ref. 77)

$$\begin{aligned} |L(\tilde{T}) - L(T)| &\leq \|T\| (LLK(\cdot, \cdot)) \\ &- \{LL_i K(\cdot, \cdot)\}^T \{L_i L_j K(\cdot, \cdot)\} \{LL_j K(\cdot, \cdot)\}^{-1} \end{aligned} \quad (16)$$

(The quantities $L_i L_j K(\cdot, \cdot)$, $L_i K(\cdot, P)$, $LLK(\cdot, \cdot)$ are what in a statistical framework would be called the covariance between the measured quantities m_i, m_j , the covariance between m_i and the value of T in the point P , the variance of $L(T)$, respectively. So the eq. (14) - (16) have there well-known counterparts in the theory of estimation or prediction.)

The main problem will naturally be the computation of the quantities $L_i L_j K(\cdot, \cdot)$, $L_i K(P, Q)$ etc. Here it has in actual applications been necessary to work with Hilbert spaces of functions harmonic down to a sphere totally enclosed in the Earth. (This sphere is the so-called Bjerhammar sphere). This gives a good possibility for choosing reproducing kernels well suited for numerical calculations. Unfortunately T will not be an element of such spaces, so the inequality (16) can not be used. On the other hand the inequality has anyway proved to be useful when the right hand side with $\|T\|$ equal to a constant is interpreted as a standard deviation.

When the observations contain errors we may instead of minimizing the norm of T minimize

$$\lambda_1 \|\tilde{T}\|^2 + \lambda_2 \{n_i\}^T \{P_{ij}\}^{-1} \{n_j\}. \quad (17)$$

This will lead to a representation of \tilde{T} as given by eq. (14), but the coefficients of the normal equations will be

$$\{L_i L_j K(\cdot, \cdot) + \frac{\lambda_2}{\lambda_1} P_{ij}\}. \quad (18)$$

From this it is clear that the estimate \tilde{T} will depend on λ_1, λ_2 , as well as on the inner product

(or norm), because the inner product determines the reproducing kernel.

If we finally will have to use an observation equation similar to eq. (8), i.e.

$$\sum_{k=1}^M A_{ki} X_k + L_i(T) + n_i = m_i, \quad (19)$$

we are back to a problem which is very similar to the combined least squares-minimum norm adjustment problem discussed in Section 3. The minimum condition to be fulfilled now is

$$\begin{aligned} \lambda_1 \|\tilde{T}\|^2 + \sum_{k=1}^M q_k X_k^2 \\ + \lambda_2 \{n_i\}^T \{P_{ij}\}^{-1} \{n_j\} = \min, \end{aligned} \quad (20)$$

which contain $M+2$ arbitrary constants: $\lambda_1, \lambda_2,$

q_1, \dots, q_M . The solution is for $\lambda_1 = \lambda_2 = 1,$
 $q_1 = q_2 = \dots = q_M = 0$ given in for example (Ref. 37).

This similarity between collocation and least squares adjustment methods has caused much confusion. Several reports and papers have been devoted to clearing up the clouds, see (Refs. 24, 81, 23, 4, 62). In (Ref. 14) a general scheme for the classification of different adjustment and collocation "setups" have been given.

The presentation of the two methods given here seems in all main points to agree with (Ref. 60).

5. LEAST SQUARES COLLOCATION

It is obvious that both in the combined least squares-minimum norm adjustment model and in the (minimum norm) collocation model the choice of a suitable norm is extremely important. Besides the purely mathematically defined norms (cf. eq. (1a, b)), another choice is possible which in a certain sense assures an optimal interpolation and prediction property.

Let us write eq. (14) as

$$\begin{aligned} \tilde{T}(P) &= \{L_i K(P, \cdot)\}^T \{L_i L_j K(\cdot, \cdot)\}^{-1} \{m_j\} \\ &= \sum_{j=1}^N b_j m_j \end{aligned} \quad (21)$$

with

$$\{b_j\} = \{L_i L_j K(\cdot, \cdot)\}^{-1} \{L_i K(P, \cdot)\}. \quad (22)$$

Then we see that the computed approximative value of $T(P)$, namely $\tilde{T}(P)$, is determined as a linear combination of the observed quantities. Suppose we require that the minimum value of the mean value of the squared approximation error,

$(T(P) - \tilde{T}(P))^2$, taken over the surface of the Earth (where the observation points move as well), is attained. Then it can be proved, cf. (Ref. 17), that the reproducing kernel to be used is the so-

called empirical covariance function. In order to achieve this conclusion we will have to work in spherical approximation. This has as its consequence that the series development of T as given by eq. (2) is convergent down to the surface of the Earth (which is approximated by a mean Earth sphere with radius R).

Then

$$K(P, Q) = \text{cov}(P, Q) \\ = \sum_{i=0}^{\infty} \sigma_i \left(\frac{R^2}{RR'} \right)^{i+1} P_i(\cos \psi), \quad (23)$$

with

$$\sigma_i = \left(\frac{GM}{R} \right)^2 \sum_{j=0}^i (C_{ij}^2 + S_{ij}^2), \quad (24)$$

P_i equal to the i 'th Legendre polynomial and ψ equal to the spherical distance between P and Q .

This reproducing kernel or empirical covariance function will implicitly define a norm in a Hilbert space (see (Ref. 77)) which unfortunately does not have T itself as an element, i.e. maximal error-bounds can not be given. However, mean square errors may be computed. They will have to be interpreted as mean square errors in a non-probabilistic sense, namely as mean values taken over all observation-point configurations which may be created by rotating the Earth about its center.

As it can be seen from eq. (23) and eq. (24) T must in principle be known before the reproducing kernel can be found. This problem has in practice been overcome by describing the variation of σ_i for $i \rightarrow \infty$ by a few parameters, which then may be estimated, see (Refs. 74, 44 or 19).

6. APPLICATION OF COLLOCATION AND LEAST SQUARES ADJUSTMENT

We should now be able to define what we understand by a collocation method and a least squares adjustment method:

Collocation is a method for the determination of a point in a linear vector space with an inner product (preferably a reproducing kernel Hilbert space), where the use of error-free observations will give a solution which agrees exactly with the observed quantities.

A least square adjustment method is a method for the determination of a point (f) in a finite dimensional linear vector space with an inner product, so that

$$\lambda_1 \|f\|^2 + \lambda_2 \{n_i\}^T \{P_{ij}\}^{-1} \{n_j\} = \min,$$

cf. Section 3.

The two methods may be equivalent when the vector spaces have a dimension equal to the number of observations.

Using these definitions we see that no true least squares adjustment procedures can be applied when dealing with gravity potential dependent data, because the "point", T , we want to determine is an element of an infinite dimensional space.

Hence when we anyway want to use least squares adjustment, we are faced with the difficult task of selecting an appropriate finite dimensional subspace. We also know, that our results will depend on this choice (see e.g. (Ref. 57)). The choice of different subspaces may also be one of the main reasons for the strange differences which are observed between different combined determinations of potential coefficients, Earth parameters and tracking station coordinates (see e.g. (Ref. 46, Fig. 4 and 5)).

When using collocation we have the equally difficult task of choosing an appropriate norm, and thereby a reproducing kernel. However, it seems that the use of the empirical covariance fct. (cf. Section 5) is a reasonable choice. Thus, the mentioned fact, that the anomalous potential not is an element of the corresponding Hilbert space may cause difficulties when big numbers of observations are used.

A big number of observations will in all applications of collocation cause problems, because the normal equation matrix $\{L, L, K(\cdot, \cdot)\}$ generally will be a full matrix. This problem may to a certain extent be overcome by separating the observations in groups, see (Refs. 39 and 75). When the number of observations increase so that a regular grid of observations may be formed, the use of integral formulae may be a better choice, cf. e.g. (Ref. 55).

Least squares adjustment has been applied extensively for the determination of station coordinates and parameters describing the long wavelength-part of the gravity potential, see (Refs. 20, 47), and more recently (Refs. 10, 22, 72, 5, and 79). Combined least squares and minimum norm adjustment has been used for potential coefficient determination by (Refs. 48, 49). Rapp has more recently (Refs. 51, 55) preferred to use collocation for the prediction of a global set of gravity anomalies and then compute potential coefficients by integration over the global dataset.

However, the determined station coordinates and potential coefficients are more different than what should have been expected from the claimed accuracies. These differences are clearly seen when comparing geoidal heights, obtained from doppler determined cartesian coordinates (in the WGS 72 coordinate system) and heights above sea level, with geoidal heights computed using the potential coefficients obtained e.g. by (Refs. 10 or 79).

The combined adjustment method has also been applied for the determination of zonal harmonics and resonant terms, see (Refs. 63, 64, 66, 67, 68, 70, and 57). These investigations show clearly the problems of the adjustment technique.

In several investigations the main goal has not been the determination of "long wavelength" information, but for example mean gravity anomalies, see (Refs. 56, 18, 16, 27, 53, 58, 61, 62 and 71).

Here the collocation method may be better suited than the adjustment technique because either a "down-ward continuation" or differentiation is needed and oscillations could be expected. This problem has been given much consideration in (Ref. 61).

Let us finally mention that both least squares and collocation methods may be useful for constructing local approximations to the gravity potential using altimeter data, geoid heights (from doppler determined positions) or gradiometers installed in an aircraft, contingently in combination with observations of surface gravity and deflections of the vertical, see e.g. (Refs. 6, 8, 52, 71). Using adjustment methods this requires the use of parameters able to represent high frequency information, and using collocation so-called local empirical covariance functions may be needed, see (Refs. 74, 76).

7. CONCLUSION

The two methods, collocation and least square adjustment, are both very useful for the handling of the very heterogeneous dataset which space research techniques have made available. Thus it seems that the differences between different solutions need to be cleared up.

As pointed out earlier in the paper several choices will have to be made (of parameters, weights and norms) before the two methods can be applied. It is therefore recommended that the influence of these choices are investigated, so that the most reliable gravity potential can be extracted from the available data.

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