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Least-Squares Collocation and the Gravitational Inverse Problem

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Abstract. The paper presents a unified least-squares method (collocation) which encompasses least-squares adjustment and least-squares prediction. This method is being applied to the determination of the terrestrial gravitational field and of geodetic position by combining data of different kind. The relationship between this method and geophysical inverse problems is discussed.

Key words: Geodesy – Gravity field – Inverse problems.

1. Introduction

The determination of the earth's external gravitational field from geodetic, gravimetric, and satellite data may be formulated as a linear inverse problem that is mathematically quite similar to other geophysical inverse problems, for instance to the determination of the internal structure of the earth from seismic and other data.

The gravitational inverse problem is likewise underdetermined. The external gravitational field requires for a complete description an infinite number of parameters, for instance, the set of all coefficients in the expansion of the external gravitational potential in spherical harmonics. This infinite number of parameters is to be determined from a finite number of observations, which is clearly an underdetermined problem.

During the last years, geodesists have worked out a comprehensive technique for the determination of the gravitational field and of geodetic position, called least-squares collocation. It has developed from two-sources: least-squares adjustment, which has been classical in land surveying and geodesy, and least-squares prediction, which is being used for some years for automatic interpolation of gravity anomalies and similar quantities. Least-squares collocation may be considered as a synthesis of adjustment and prediction to provide a unified method for determining geometrical and physical parameters related to the figure of the earth and its gravity field.

Least-squares collocation has many features in common with other geophysical inversion techniques. It may, therefore, be of interest to give a brief review of collocation, exhibiting cross-connections to geophysical inversion methods. The reader will find more information and references in (Brosowski and Martensen, 1975; Grafarend, 1975; Moritz, 1973).

2. Determination of Spherical Harmonics

We shall start with an example for which the relation with geophysical inversion problems is particularly obvious: the determination of the spherical-harmonic expansion for the gravitational potential from satellite data.

This expansion may be written as

$$V(r, \theta, \lambda) = \frac{GM}{r} \left[1 - \sum_{n=2}^{\infty} \left(\frac{a}{r}\right)^n J_n P_n(\cos \theta) - \sum_{n=2}^{\infty} \sum_{m=1}^n \left(\frac{a}{r}\right)^n P_{nm}(\cos \theta) (J_{nm} \cos m\lambda + K_{nm} \sin m\lambda) \right]. \quad (1)$$

Here V denotes the external gravitational potential of the earth; r (radius vector), θ (polar distance = co-latitude) and λ (longitude) are spherical coordinates; $P_n(\cos \theta)$ and $P_{nm}(\cos \theta)$ are Legendre functions – zonal and tesseral, respectively –; G denotes the gravitational constant, M the total mass of the earth, a the earth's equatorial radius; and J_n , J_{nm} and K_{nm} are coefficients to be determined empirically.

An arbitrary measurement to a satellite (a photographically observed direction, an electronically measured distance or range-rate, etc.) is obviously a function of these parameters J_n , J_{nm} and K_{nm} , since the orbit of the satellite is influenced by the gravitational field:

$$L = f(J_n, J_{nm}, K_{nm}).$$

To linearize this function f one introduces approximate values for these parameters as reference values and expands by Taylor's theorem. This gives an expression linear in the differences δJ_n , δJ_{nm} , δK_{nm} (actual minus reference values), of the form

$$L = L^0 + \sum_{r=1}^{\infty} l_r s_r, \quad (2)$$

where L^0 is the function f evaluated in terms of the reference values; the s_r are the differences δJ_n , δJ_{nm} , δK_{nm} in some linear order, e.g. $s_1 = \delta J_{20}$, $s_2 = \delta J_{21}$, $s_3 = \delta K_{21}$, $s_4 = \delta J_{22}$, $s_5 = \delta K_{22}$, $s_6 = \delta J_{30}$, etc.; and the l_r are coefficients (the partial derivatives of L with respect to s_r).

If we have q observations L and denote the differences $L - L^0$ by x_i , then we obtain q equations of type (2):

$$\sum_{r=1}^{\infty} b_{ir} s_r = x_i \quad (i = 1, 2, \dots, q). \quad (3)$$

In matrix notation this may be written as

$$\mathbf{B}\mathbf{s} = \mathbf{x}. \quad (4)$$

A general solution of this underdetermined system (assumed full-rank) is

$$\mathbf{s} = \mathbf{K}\mathbf{B}^T(\mathbf{B}\mathbf{K}\mathbf{B}^T)^{-1} \mathbf{x}, \quad (5)$$

where \mathbf{K} is an (infinite) square matrix such that the occurring infinite sums converge and that $\mathbf{B}\mathbf{K}\mathbf{B}^T$ is a regular $q \times q$ matrix; otherwise \mathbf{K} is arbitrary.

The matrix

$$\mathbf{B}^- = \mathbf{K}\mathbf{B}^T(\mathbf{B}\mathbf{K}\mathbf{B}^T)^{-1} \quad (6)$$

is a right (generalized) inverse of \mathbf{B} ; the solution (5) obviously satisfies (4). Less obvious but also well known from the theory of generalized inverses (cf. Bjerhammar, 1973, p. 116) is the fact that the solution (5) satisfies the minimum condition

$$\mathbf{s}^T \mathbf{K}^{-1} \mathbf{s} = \text{minimum}, \quad (7)$$

provided the matrix \mathbf{K}^{-1} exists in an appropriate sense. (In general, operations with infinite matrices are formally identical to ordinary matrix operations provided the infinite sums converge.)

Usually the measurements x_i are affected by unknown observational errors, denoted by n_i ; the notation follows the terminology of time series: “s” stands for “signal”, and “n” for “noise”. Then (3) is to be replaced by

$$\sum_{r=1}^{\infty} b_{ir} s_r + n_i = x_i, \quad (8)$$

or in matrix notation:

$$\mathbf{B}\mathbf{s} + \mathbf{n} = \mathbf{x}. \quad (9)$$

An appropriate minimum condition, replacing (7), is now

$$\mathbf{s}^T \mathbf{K}^{-1} \mathbf{s} + \mathbf{n}^T \mathbf{D}^{-1} \mathbf{n} = \text{minimum}, \quad (10)$$

where \mathbf{K} and \mathbf{D} can be interpreted statistically as *covariance matrices*: \mathbf{K} is the covariance matrix of the “signal” \mathbf{s} , that is, of the spherical-harmonic coefficients, and \mathbf{D} is the covariance matrix of the “noise” \mathbf{n} , that is, of the observational errors.

The solution of (9) under the minimum condition (10) is readily found to be

$$\mathbf{s} = \mathbf{K}\mathbf{B}^T(\mathbf{B}\mathbf{K}\mathbf{B}^T + \mathbf{D})^{-1} \mathbf{x}. \quad (11)$$

The mathematical model (9) and the solution (11) have also been suggested for geophysical inverse problems (cf. Wiggins, 1972, pp. 260–1). This solution has remarkable mathematical and numerical properties, especially stability.

For the determination of the earth’s gravitational field this model has still other advantageous features. The covariance matrices \mathbf{K} and \mathbf{D} are not just auxiliary mathematical quantities introduced in order to obtain a convenient solution of (9), but they admit of a physical definition in terms of the statistics of the anomalous gravity field and are, in principle, determinable by observation. Furthermore, the determination of \mathbf{s} by (11) is optimal in the sense that it has the smallest standard (r.m.s.) error possible on the basis of the given data. It is, more-

over, perfectly consistent with apparently quite different techniques, for instance, least-squares interpolation of gravity anomalies. All these techniques fit into the general framework of least-squares collocation to be considered in Sections 4 and 5.

3. Least-Squares Interpolation

Consider the following problem of a quite different nature. Let the gravity anomaly Δg (measured gravity g minus normal gravity γ) be given at q points P_1, P_2, \dots, P_q at the earth's surface, represented e.g. by a sphere; to interpolate Δg at another point P of the sphere.

If we consider the Δg -field as a stochastic process on the sphere, we may apply the theory of least-squares interpolation of stochastic processes. The resulting formula is (cf. Heiskanen and Moritz, 1967, p. 268):

$$\Delta g_P = [C_{P1} \ C_{P2} \ \dots \ C_{Pq}] \begin{bmatrix} C_{11} & C_{12} & \dots & C_{1q} \\ C_{21} & C_{22} & \dots & C_{2q} \\ \vdots & & & \vdots \\ C_{q1} & C_{q2} & \dots & C_{qq} \end{bmatrix}^{-1} \begin{bmatrix} \Delta g_1 \\ \Delta g_2 \\ \vdots \\ \Delta g_q \end{bmatrix}. \tag{12}$$

Here Δg_P denotes the gravity anomaly to be interpolated at point P ; $\Delta g_1, \Delta g_2, \dots, \Delta g_q$ are the gravity anomalies given at P_1, P_2, \dots, P_q , and the C_{Pi} and C_{ik} are covariances which can all be expressed in terms of *one* covariance function $C(\psi)$, where ψ denotes the spherical distance:

$$C_{Pi} = C(\psi_{Pi}), \tag{13}$$

$$C_{ik} = C(\psi_{ik}), \tag{14}$$

ψ_{Pi} being the spherical distance between P and P_i , and ψ_{ik} between P_i and P_k (cf. Runcorn, 1967, pp. 1437-8).

Is there any relation between the ideas of Section 2 and the present case? The problems are as different as they can be. The only indication for a possible interrelation is the minimum standard error property, which holds for (11) as well as for Δg_P , minimum standard error being the condition from which (12) derived.

Let us assume that we want to solve our present interpolation problem on the basis of the ideas of the preceding section. In this case we should have to express Δg in terms of spherical harmonics:

$$\Delta g = \sum_{n=2}^{\infty} c_n P_n(\cos \theta) + \sum_{n=2}^{\infty} \sum_{m=1}^n (c_{nm} \cos m\lambda + d_{nm} \sin m\lambda) P_{nm}(\cos \theta). \tag{15}$$

This is, in fact, possible, the c_n, c_{nm} and d_{nm} being proportional to $\delta J_n, \delta J_{nm}$ and δK_{nm} , respectively (Heiskanen and Moritz, 1967, p. 108). There exists, therefore, a relation

$$\Delta g(\theta, \lambda) = \sum_{r=1}^{\infty} B_r(\theta, \lambda) s_r, \tag{16}$$

where $B_r(\theta, \lambda)$ are certain functions of (θ, λ) , obviously related to the Legendre functions.

It is now possible to write Equation (16) for all given points P_i , obtaining q Equations (3) with $x_i = \Delta g_i$ and $b_{ir} = B_r(\theta_i, \lambda_i)$. The linear equation system so obtained may be solved by (5); we assume that there are no measuring errors, whence $\mathbf{D} = 0$. The infinitely many quantities s_r thus found are substituted into (16), written for point P , to obtain Δg_P .

It is clear that this solution is totally impractical, but if we would try it and succeed in performing correctly all the numerical operations, what would we get? Precisely the same result as by using (12) (provided we operate with correct covariances and disregard convergence problems)!

The reason for this equivalence will be made clear in the following section. Here we remark only that Equation (12) contains only finite matrices and vectors, whereas (5) deals with infinite matrices and vectors. The reason is that (12) involves covariance *functions*. Since a function, as element of a Hilbert space, is in some sense equivalent to an infinite vector (e.g. composed of Fourier coefficients), the infinite number of degrees of freedom is, so to speak, built into the covariance function and does not explicitly appear.

Finally I should like to point out another feature of the interpolation formula (12), namely *locality*. Assume that the data points P_i all lie in a certain small region. Then one cannot hope, from these local data, to obtain meaningful estimates for the spherical-harmonic coefficients, which form the vector \mathbf{s} of Section 2. Nevertheless, the interpolated value Δg_P according to (12) will be quite reliably determined provided P is closely surrounded by data points P_i . Thus Equation (12) works in a local fashion, in contrast with (5).

In the terminology of Backus and Gilbert (1968), the local interpolation formula (12) expresses a *deltalike functional*.

4. The Many Facets of Collocation

The question now arises: What is the common background, if any, for the methods of Sections 2 and 3? Is there a general mathematical model, of which these methods are only special cases?

In fact, there is such a general model. If we subtract a suitably defined "normal" (ellipsoidal) gravitational field from the actual gravitational field of the earth, then the residual field will be quite small; it is called *anomalous field*, or disturbing field. This holds for all field quantities, not only for the potential: quantities pertaining to the anomalous field are, for instance, the disturbing potential T , gravity anomalies Δg , geoidal heights N , or deflections of the vertical ξ, η . All these quantities are related to each other by linear differential or integral operations, such as Stokes integral expressing N in terms of Δg . These operations may be considered as linear operators or linear functionals in a suitable Hilbert space.

The basic idea is now to consider the anomalous potential T , which is small, fluctuates irregularly and has, in some sense, zero average, as a stationary stochastic process on the sphere, and the other anomalous field quantities as other stochastic processes derived from the T field by linear operations mentioned.

These stochastic processes possess covariance function which are related by analogous linear operations ("propagation of covariances") to a basic function,

for which we may take the covariance function $K(P, Q)$ of the anomalous potential T . This function can be developed in spherical harmonics as

$$K(P, Q) = \sum_{n=0}^{\infty} k_n \left(\frac{r_0^2}{r_P r_Q} \right)^{n+1} P_n(\cos \psi), \tag{17}$$

where r_P and r_Q are the radius vectors of the spatial points P and Q and ψ is the angle between these two radius vectors; $P_n(\cos \psi)$ are Legendre polynomials, r_0 is a constant slightly smaller than the mean radius of the earth, and the k_n are non-negative coefficients. This expression shows that $K(P, Q)$ is harmonic, satisfying Laplace's equation at both points P and Q .

Any quantity of the anomalous gravity field may thus be considered as a random "signal" s . Assume that a certain number q of such quantities, which form a vector \mathbf{x} , has been measured and that we want to derive from them a set of p other, unknown, quantities of the anomalous gravity field, which form the vector \mathbf{s} . The solution of this problem is given by the fundamental *Wiener-Kolmogorov prediction formula*

$$\mathbf{s} = \mathbf{C}_{sx} \mathbf{C}_{xx}^{-1} \mathbf{x} \tag{18}$$

(cf. Liebelt, 1967, p. 138; he calls it Gauss-Markoff theorem). In statistical terms, this is the *linear minimum variance unbiased estimate* for the quantities forming the vector \mathbf{s} . The matrices \mathbf{C}_{sx} and \mathbf{C}_{xx} are covariance matrices that are interrelated by covariance propagation mentioned above.

The formula (18) has very nice mathematical properties which are unique indeed, being related to geometrical features of Hilbert space:

- minimum variance, that is, best possible accuracy available on the basis of the given data;

- invariance with respect to linear operations; this ensures that all quantities \mathbf{s} so obtained are mutually compatible and refer to one and the same gravity field;

- both vectors \mathbf{x} and \mathbf{s} may comprise arbitrary, even heterogeneous, quantities of the anomalous gravity field;

- the measurements \mathbf{x} may even be affected by random errors ("noise"); formula (18) will still hold provided the covariance matrix \mathbf{C}_{xx} is modified by adding the corresponding covariance matrix of the noise.

Equation (12) is now readily recognized as a special case of (18), if all components of the observation vector \mathbf{x} are gravity anomalies Δg_i and if the vector \mathbf{s} consists only of one component Δg_P .

But also (11) is derivable from (18). Let \mathbf{s} be the infinite vector of the spherical-harmonic coefficients, as in Section 2, and let the covariance matrix of this vector be known and denoted by \mathbf{K} ; this matrix is found to be a diagonal matrix whose diagonal elements are proportional to k_n in (17). Let further the covariance matrix of the measuring errors \mathbf{n} be denoted by \mathbf{D} , and let \mathbf{s} and \mathbf{n} be uncorrelated. Then the application of covariance propagation to (9) gives easily

$$\mathbf{C}_{xx} = \mathbf{KKB}^T + \mathbf{D}, \tag{19}$$

$$\mathbf{C}_{sx} = \mathbf{KB}^T, \tag{20}$$

whence (18) in fact becomes (11).

Thus the theory of stochastic processes provides a very convenient mathematical formalism and terminology. How seriously the statistical interpretation is to be taken, is a matter of controversy and also of personal taste. It is possible largely to play down the statistical aspects, emphasizing Hilbert space geometry and considering the covariance function as a kernel function in Hilbert space, as Krarup did in his fundamental paper (1969). (There are interesting parallels with Backus' (1970) Hilbert space treatment of geophysical inversion problems.)

The statistical and the Hilbert space approach are mathematically completely equivalent (isomorphic). Both approaches provide important insight, and they complement each other, rather than competing with each other. To avoid the impression that the present method "messes up every thing statistically", we look at it from yet another angle, which shows that we do have an underlying completely "clean" analytic model.

We represent the anomalous gravity potential T at some point P as a linear combination of sufficiently many suitable base functions $\phi_i(P)$:

$$T(P) = \sum_{i=1}^q b_i \phi_i(P). \quad (21)$$

The base functions ϕ_i are to be harmonic functions of a simple analytic form; b_i are numerical coefficients.

Assume that we have q errorless data, which are linear functionals of T , such as gravity anomalies, deflections of the vertical, spherical-harmonic coefficients, etc. The problem is to fit the expression (21) to the data, so that the q given functionals are exactly reproduced. This is the principle of *collocation*, which is frequently used in numerical mathematics (cf. Collatz, 1966).

Once the functions ϕ_i are given, the q coefficients b_i are completely determined by the q data, supposed independent. Depending on the choice of the functions ϕ_i , the interpolation error using the finite approximation (21) will vary. Now the functions ϕ_i are determined in such a way that the r.m.s. interpolation error m_p is minimized; this accounts for the name "*least-squares collocation*" for the method described in the present paper.

From this principle one obtains the explicit solution

$$\phi_i(P) = C(P, x_i), \quad (22)$$

which is the covariance between $T(P)$ and the measurement x_i . It is a function of point P , for which a suitable analytical expression should be used. The coefficients b_i , which form the vector \mathbf{b} , are determined from the equation

$$\mathbf{b} = \mathbf{C}_{xx}^{-1} \mathbf{x}, \quad (23)$$

where \mathbf{C}_{xx} is the autocovariance matrix of the observation vector $\mathbf{x} = (x_i)$.

Thus, with errorless data, least-squares collocation determines the analytical form of the functions ϕ_i by the requirement of optimal accuracy, whereas the data are exactly reproduced.

If the data are affected by measuring errors, then the requirement $m_p = \text{minimum}$ determines simultaneously

- (1) the best analytical expression for the functions ϕ_i and
- (2) the best values for the coefficients b_i .

In this case, the mathematical expressions are the same as before, (22) and (23). The measuring errors have no influence on the choice of ϕ_i by (22), so that ϕ_i again represent pure signal covariance functions, that is, analytical and harmonic functions; again the least-squares principle helps only to single out the most suitable analytical expression for the base functions ϕ_i among the many possible choices.

Where statistics enters directly, is the determination of the coefficients b_i , which is done in such a way that the effect of the measuring errors is minimized; in statistical terminology, we have a “best linear estimate”: an unbiased linear estimate of minimum variance, as we have already mentioned.

Expressions analogous to (21) may be given for any other quantity of the anomalous gravity field, such as geoidal heights, deflections of the vertical, gravity anomalies, etc. The coefficients b_i remain the same since they depend only on the data \mathbf{x} by (23); what changes are the base functions ϕ_i ; the new base functions are derived by simple analytical operations such as differentiation since a linear operation performed on (21) acts on the base functions ϕ_i . This is, of course, covariance propagation as mentioned above, which is now seen to carry the precise mathematical structure of the terrestrial gravitational field.

In fact, (21) together with (23) is the same as the prediction formula (18), so that we have only been looking at the same mathematical model from different angles. For lack of time it is impossible here to consider the treatment in terms of Hilbert space with kernel functions (Krarup, 1969), which provides still another aspect.

If esthetic appeal in science is characterized by a combination of basic simplicity, richness of mathematical structure, and practical usefulness, then least-squares collocation might present itself as a candidate for such a qualification.

5. Inclusion of Systematic Parameters

So far we have assumed that we deal only with quantities that have zero average (zero statistical expectation), such as the elements of the anomalous gravitational field. This restriction must be removed if the least-squares collocation is to be applicable to more general geodetic problems.

We shall, therefore, consider the following model:

$$\mathbf{x} = \mathbf{A}\mathbf{X} + \mathbf{s} + \mathbf{n}, \quad (24)$$

where the vector \mathbf{x} comprises the measured quantities and \mathbf{s} are the signal and noise parts, as before. The new component is $\mathbf{A}\mathbf{X}$, where the vector \mathbf{X} comprises systematic, non-random parameters, and \mathbf{A} is a known matrix.

This model is general enough to encompass all conceivable geodetic measurements. In fact, any geodetic measurement may be split up, according to (24), into 3 parts:

1. a systematic part $\mathbf{A}\mathbf{X}$ involving, on the one hand, the ellipsoidal reference system and, on the other hand, other parameters and systematic errors (original non-linear functions are thought to have been linearized by Taylor's theorem);
2. a random part \mathbf{s} expressing the effect of the anomalous gravity field; and
3. random measuring errors \mathbf{n} .

As an example, consider a measurement of gravity, g . Here \mathbf{AX} represents normal gravity γ , as well as systematic errors such as gravimeter drift; \mathbf{s} is the gravity anomaly Δg ; and \mathbf{n} stands for the measuring error.

The formulas for estimating \mathbf{X} and \mathbf{s} may be derived from either of two different, but equivalent, minimum principles:

1. From a least-squares principle corresponding to (10);
2. From the condition of minimum variance (least standard errors of estimated

\mathbf{X} and \mathbf{s}).

The results are

$$\mathbf{X} = (\mathbf{A}^T \mathbf{C}_{xx}^{-1} \mathbf{A})^{-1} \mathbf{A}^T \mathbf{C}_{xx}^{-1} \mathbf{x}, \quad (25)$$

$$\mathbf{s} = \mathbf{C}_{sx} \mathbf{C}_{xx}^{-1} (\mathbf{x} - \mathbf{AX}). \quad (26)$$

The first equation is analogous to classical least-squares adjustment by parameters, except that the covariance matrix \mathbf{C}_{xx} includes now the covariances of the signal as well as those of the measuring errors. The second equation is an obvious generalization of (18) to the case in which the expectation of \mathbf{x} is \mathbf{AX} rather than zero.

These formulas are an extension of the corresponding problem for time series (Grenander and Rosenblatt, 1957, p. 87).

The present method may be regarded as a combination of least-squares adjustment and least-squares prediction into a unified scheme, which makes possible the use of all geodetic data – classical angle and distance measurements, gravity measurements, satellite data of different kind, etc. – to obtain the geometrical position of points of the earth's surface as well as the gravitational field.

As an idealization, we might assume that *all* geodetic data available at the present time are combined by (25) and (26) into a single solution for the earth's gravity field. As a matter of fact, this cannot be directly realized in practice because it would involve the inversion of an excessively large \mathbf{C}_{xx} matrix.

In practice, the number of data to be combined is limited by the size of matrix that can be inverted by the computer. This presupposes suitable representative selection of the data and some working "from the large to the small" in several steps.

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