Least-Squares Collocation

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Least-squares collocation is a mathematical technique for determining the earth's figure and gravitational field by a combination of heterogeneous data of different kinds. The same formulas may be interpreted in very different ways: as the solution of a geophysical inverse problem, as a statistical estimation method combining least-squares adjustment and least-squares prediction, and as an analytical approximation to the earth's potential by means of harmonic functions. The present review article attempts a unified presentation of the subject with emphasis on theory.

INTRODUCTION

Since the review articles by *Kaula* [1963, 1967] the subject of estimating the earth's gravitational field from measurements of different types, quality, and distribution has developed considerably. Least-squares collocation has started from the subject of interpolation of gravity anomalies by least-squares prediction and has been generalized to arbitrary data. The statistical origin of collocation has sometimes overshadowed the fact that this method can also be considered as a purely analytical approximation method.

The present article attempts a review of the subject from a theoretical point of view. The subject is first approached from approximation theory, before embarking on statistical interpretation. The list of references is intended to give a representative sample of all principal trends. Its object is to guide the readers, rather than provide a complete documentation. It is essentially restricted to literature published within the last 10 years; earlier literature is given by *Kaula* [1963, 1967] and *Heiskanen and Moritz* [1967].

The fundamental publication on collocation is a paper by *Krarup* [1969]; a comprehensive elementary presentation is given by *Moritz* [1973]; a compact review paper from the stochastic process point of view with a very complete bibliography is by *Grafarend* [1976]; and a good picture of the present status is provided by a collection of lectures presented at a summer school in Ramsau, Austria, in August 1977 [*Moritz and Sünkel*, 1978].

1. APPROXIMATE REPRESENTATION OF THE EARTH'S GRAVITATIONAL FIELD

The earth's external gravitational potential V is conventionally split up as follows:

$$V = V_R + T \tag{1}$$

where V_R, the reference potential or normal potential, is usually taken as the external potential of a reference ellipsoid, which is given by a simple closed analytical expression [cf. *Heiskanen and Moritz*, 1967, p. 66]; thus V_R can be considered known. The quantity

$$T = V - V_R \tag{2}$$

called the disturbing potential, or the anomalous potential, is small but quite irregular. Therefore its analytical representation poses some problems, with which we shall be concerned in the following.

Clearly, such an analytical representation can only be approximate. We shall try to approximate T by a linear combination f of suitable base functions $\phi_1, \phi_2, \phi_3, \cdots, \phi_q$:

$$T(P) \doteq f(P) = \sum_{k=1}^{q} b_k \phi_k(P) \tag{3}$$

P denoting the space point at which these functions are being considered and b_k designating suitable coefficients.

Since T is harmonic outside the earth's surface, it is appropriate to select as base functions ϕ_k also harmonic functions, satisfying Laplace's equation

$$\Delta \phi_k = 0 \tag{4}$$

Otherwise, many different choices are possible. The ϕ_k may, for instance, be spherical harmonics or the potential of point masses suitably distributed below the earth's surface. The coefficients b_k are chosen so as to satisfy certain conditions.

Interpolation. Assume, for instance, that we are given errorless values of T at q space points P_i. Then we may postulate that the approximation f to T, as given by (3), exactly reproduces T at the q given points. On putting

$$f(P_i) = T(P_i) = f_i \qquad i = 1, 2, \cdots, q \tag{5}$$

we thus have the conditions

$$\sum_{k=1}^{q} A_{ik} b_k = f_i \qquad A_{ik} = \phi_k(P_i) \tag{6}$$

They form q linear equations for the q unknowns b_k, which can be solved uniquely provided they are linearly independent.

Collocation. A generalization of the interpolation problem is the case in which q values of linear functionals $L_1T, L_2T, \cdots, L_qT$ of T are to be reproduced. Such functionals are, for instance, values of deflection of the vertical components

$$\xi = -\frac{1}{G}\frac{\partial T}{\partial x} \qquad \eta = -\frac{1}{G}\frac{\partial T}{\partial y} \tag{7}$$

and gravity anomalies

$$\Delta g = -\frac{\partial T}{\partial z} - \frac{2}{R} T \tag{8}$$

at certain data points; here xyz represents a local coordinate system, the z axis being vertical and directed upward and the x axis pointing north, and $R = 6370$ km is the mean radius of the earth.

On putting

$$L_i f = L_i T = l_i \tag{9}$$

Paper number 8R0304.
0034-6853/78/038R-0304$06.00

we thus get from (3)

$$\sum_{k=1}^{q} B_{ik} b_k = l_i \qquad B_{ik} = L_i \phi_k \tag{10}$$

which is a $q \times q$ linear system for b_k quite similar to (6). This method for fitting an analytical approximation to q given functionals is called collocation and is frequently used in numerical mathematics [cf. *Collatz*, 1966, p. 29].

It is clear that interpolation is a special case of collocation if the functionals $L_i f$ are the 'evaluation functionals' $f(P_i)$.

We thus see that in both interpolation and collocation, for any assumed system of base functions ϕ_k the determination of the coefficients b_k always involves the solution of a $q \times q$ system of linear equations (which will, in general, not be symmetric).

2. Least-Squares Interpolation and Collocation

Least-squares interpolation. The base functions $\phi_i(P)$ for interpolation may be selected in such a way that the rms interpolation error m_P is minimized; here m_P is defined by

$$m_P^2 = M\{\epsilon_P^2\} \tag{11}$$

where

$$\epsilon_P = T(P) - f(P) \tag{12}$$

is the local interpolation error (it is zero at the q data points P_i). The symbol M denotes a suitable mean or average (see below).

The condition

$$m_P = \min \tag{13}$$

leads to

$$\phi_k(P) = K(P, P_k) \tag{14}$$

where the covariance function $K(P, Q)$ is defined by

$$K(P, Q) = M\{T(P)T(Q)\} \tag{15}$$

M being the averaging operator already used above. Thus in (6),

$$A_{ik} = K(P_i, P_k) = C_{ik} \tag{16}$$

and we can solve for b_k and substitute into (3). On putting

$$\phi_k(P) = K(P, P_k) = C_{Pk} \tag{17}$$

the result is

$$f(P) = [C_{P1} \ C_{P2} \ \cdots \ C_{Pq}] \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1q} \\ C_{21} & C_{22} & \cdots & C_{2q} \\ \vdots & \vdots & & \vdots \\ C_{q1} & C_{q2} & \cdots & C_{qq} \end{bmatrix}^{-1} \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_q \end{bmatrix} \tag{18}$$

This least-squares interpolation formula is frequently used for gravity interpolation, on taking $f = \Delta g$ instead of T; compare with the derivation of *Heiskanen and Moritz* [1967, p. 268]. It is, of course, nothing but the Wiener-Kolmogorov prediction formula, well known from the theory of stochastic processes [cf. *Grafarend*, 1975*a*; *Liebelt*, 1967, p. 138].

Least-squares collocation. Here the minimum principle (13), the least rms interpolation error, leads to

$$\phi_k(P) = L_k{}^Q K(P, Q) \tag{19}$$

where $L_k{}^Q$ means that the linear functional L_k is applied to the variable Q. Thus in (10),

$$B_{ik} = L_i{}^P L_k{}^Q K(P, Q) = C_{ik} \tag{20}$$

On putting

$$\phi_k(P) = L_k{}^Q K(P, Q) = C_{Pk} \tag{21}$$

we get formally the same formula (18) as before but with $f_1, f_2, \cdots, f_q$ replaced by $l_1, l_2, \cdots, l_q$:

$$f(P) = [C_{P1} \ C_{P2} \ \cdots \ C_{Pq}] \begin{bmatrix} C_{11} & C_{12} & \cdots & C_{1q} \\ C_{21} & C_{22} & \cdots & C_{2q} \\ \vdots & \vdots & & \vdots \\ C_{q1} & C_{q2} & \cdots & C_{qq} \end{bmatrix}^{-1} \begin{bmatrix} l_1 \\ l_2 \\ \vdots \\ l_q \end{bmatrix} \tag{22}$$

The application of the simple least-squares prediction formula (18) to problems involving the gravitational field is rather limited, essentially to the interpolation of gravity anomalies and similar tasks. On the other hand, the least-squares collocation formula has a considerably wider scope of application because it involves as data arbitrary linear functionals of T. In fact, geodetic data are of many different types: horizontal and vertical angles, distances, gravity measurements, astronomical observations of latitude and longitude, satellite observations of many kinds, second-order gravity gradients, etc. All these geodetic data obviously share the property that they depend on the earth's gravitational field; therefore on linearization all of them may be expressed as linear functionals of the anomalous potential T, for example, (7) and (8), so as to serve as data for an optimal determination of T by (22).

Least-squares interpolation and collocation share with all representation methods of type (3) the disadvantage that a (usually large) $q \times q$ matrix has to be inverted; it has, however, the advantage that the matrix to be inverted here, being a covariance matrix, is symmetric, in contrast to the general case of a nonsymmetric matrix in (6) and (10).

So far, we have supposed that the data are errorless. It is easy, however, to generalize least-squares collocation to the case in which there are random measuring errors and also systematic parameters to be determined. This will be done in section 4; in section 3 we shall consider the problem of the covariance function, which obviously plays a fundamental role here.

3. Covariance Functions

As we have seen, the base functions (17) and (21) are directly related to covariance functions. If a simple analytical form for $K(P, Q)$ is chosen, then the base functions will be analytically simple functions, which is desirable in many applications. In fact, the method described in the preceding section works with any function $K(P, Q)$ that is symmetric in P and Q, harmonic as a function of both P and Q, and positive definite (see below). Thus this method can be considered purely as an analytical approximation without statistical interpretation, the function $K(P, Q)$ being a kernel function in a Hilbert space with reproducing kernel [*Meschkowski*, 1962, p. 114; *Krarup*, 1969; *Tscherning*, 1975*b*, 1977].

Choosing the kernel function $K(P, Q)$ to be the covariance function of T becomes essential only if we wish to achieve minimum rms interpolation error. On the other hand, the exact covariance function of the disturbing potential T, even if it could be determined exactly, would probably not have a simple analytical form. By fitting a suitable expression to the empirical covariance data, one may hope to reconcile the two desiderata, simplicity and optimality, in a practically acceptable way.

In (15) we have introduced the covariance function as

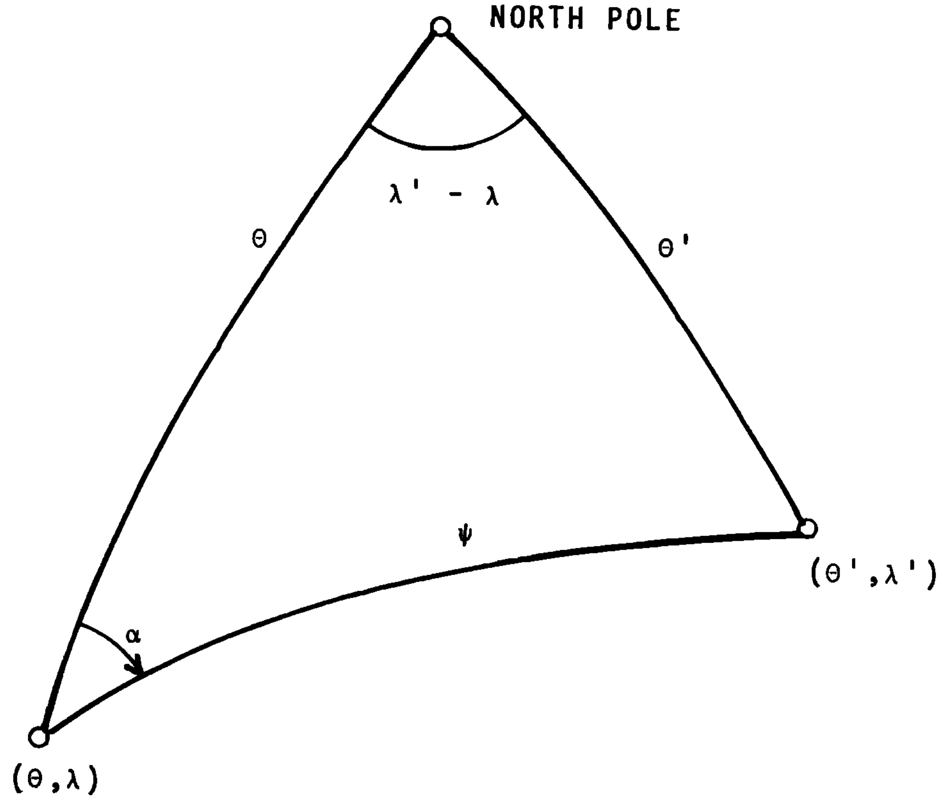

Fig. 1. The basic spherical triangle.

$$K(P, Q) = M\{T(P)T(Q)\} \tag{23}$$

If we should consider a statistical ensemble of various 'sample earths' with similar statistical properties, then we could regard M as an ensemble average or a statistical expectation. This would correspond to the interpretation of the anomalous gravitational field as a stochastic process [*Grafarend,* 1975*b*, 1976].

It may appear preferable not to introduce other sample earths and to work only with the anomalous gravitational field of the actual earth. Then the operator M must be some kind of global (or, possibly, regional) average.

We may start with the case in which both points P and Q are on the surface of a sphere $r = R$ representing a mean terrestrial sphere. If we prescribe M to be a homogeneous and isotropic operator, then the function $K(P, Q)$ will be a function only of the spherical distance ψ between P and Q:

$$K(P, Q) = K(\psi) = \frac{1}{8\pi^2} \int_{\lambda=0}^{2\pi} \int_{\theta=0}^{\pi} \int_{\alpha=0}^{2\pi} T(\theta, \lambda) \cdot T(\theta', \lambda') \sin\theta \, d\theta \, d\lambda \, d\alpha \tag{24}$$

where (θ, λ) and (θ', λ') denote points on the sphere that have a spherical distance ψ, such that (Figure 1)

$$\cos\psi = \cos\theta \cos\theta' + \sin\theta \sin\theta' \cos(\lambda' - \lambda) \tag{25}$$

Both points (θ, λ) and (θ', λ') are variable but subject to the condition that their distance ψ remains constant. The azimuth α may also be expressed in terms of (θ, λ) and (θ', λ') by well-known formulas of spherical trigonometry.

The integration over (θ, λ) in (24) expresses homogeneity, and the integration over the azimuth α denotes isotropy. The two concepts, homogeneity and isotropy, are obviously closely interrelated in the case of the sphere. The three parameters θ, λ, and α may be interpreted as three Eulerian angles of a rotation, so that the operator M defined by (24) is an average over rotation group space.

A spherical harmonic expansion of the covariance function gives

$$K(\psi) = \sum_{n=2}^{\infty} k_n P_n(\cos\psi) \tag{26}$$

where the $P_n(\cos\psi)$ are Legendre's polynomials. If the anomalous potential T on the sphere $r = R$ is likewise expanded into spherical harmonics:

$$T(\theta, \lambda) = \sum_{n=2}^{\infty} \sum_{m=0}^{n} (\bar{a}_{nm} \cos m\lambda + \bar{b}_{nm} \sin m\lambda)\bar{P}_{nm}(\cos\theta) \tag{27}$$

$\bar{P}_{nm}(\cos\theta)$ denoting the fully normalized Legendre's functions, then the coefficients k_n of K are related to the coefficients $\bar{a}_{nm}$ and $\bar{b}_{nm}$ of T by [*Kaula,* 1959]

$$k_n = \sum_{m=0}^{n} (\bar{a}_{nm}^2 + \bar{b}_{nm}^2) \tag{28}$$

[cf. *Heiskanen and Moritz,* 1967, section 7-3]; there we have considered the covariance function $C(\psi)$ of Δg instead of the covariance function $K(\psi)$ of T.

The extension of the function (26) into space outside the sphere $r = R$ follows uniquely if we note that the function $K(P, Q)$ in space must be harmonic both with respect to P and with respect to Q, i.e., it must satisfy Laplace's equation whether it is considered as a function of point P or as a function of point

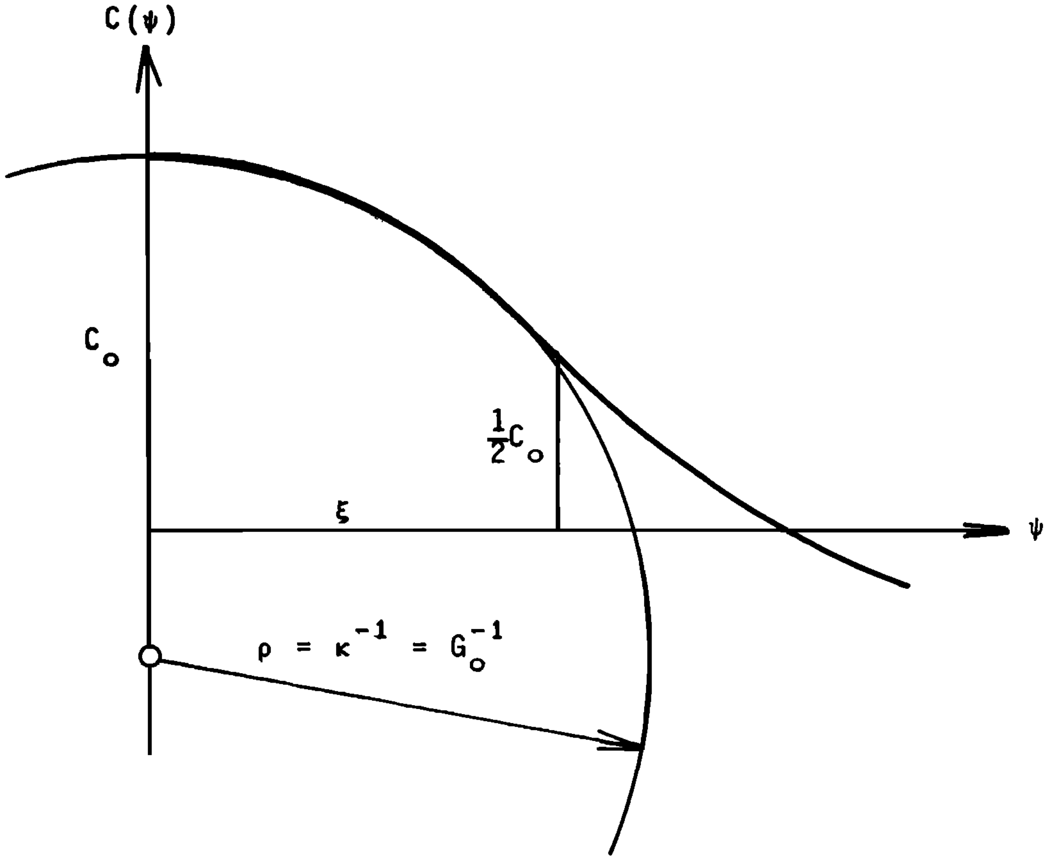

Fig. 2. Local parameters of a covariance function.

Q (this is a simple consequence of the harmonicity of T). We thus get, in space,

$$K(P, Q) = \sum_{n=2}^{\infty} k_n \left(\frac{R^2}{r_P r_Q}\right)^{n+1} P_n(\cos\psi) \tag{29}$$

r_P and r_Q being the radius vectors of points P and Q, respectively.

The corresponding covariance function of the gravity anomaly Δg is given by

$$C(P, Q) = \sum_{n=2}^{\infty} c_n \left(\frac{R^2}{r_P r_Q}\right)^{n+2} P_n(\cos\psi) \tag{30}$$

where

$$c_n = (n-1)^2 R^{-2} k_n \tag{31}$$

This follows immediately from the well-known spherical harmonic relation between T and Δg [*Heiskanen and Moritz,* 1967, p. 97] and from the fact that $r\Delta g$ is harmonic in space [*Heiskanen and Moritz,* 1967, p. 90]. In this way, from one of the functions $C(P, Q)$ and $K(P, Q)$ it is possible to compute the other.

All covariance functions, as well as all covariance matrices, must be positive definite. Positive definiteness of a function is equivalent to the nonnegativity of the spectrum [cf. *Papoulis,* 1965, p. 349]. In the case of functions defined on a sphere, the spectral representation is the expansion into spherical harmonics. Therefore positive definiteness of the functions K and C is equivalent to the nonnegativity of all coefficients k_n and c_n, which is guaranteed by (28) and (31).

Empirical determination. If the gravity anomaly Δg were known over the whole earth, then $C(P, Q)$ would be obtained by integrating the product $\Delta g(\theta, \lambda)\Delta g(\theta', \lambda')$ according to (24), with T replaced by Δg. In view of the gaps in the global gravity coverage, one resorts to suitable sampling techniques. The lower degree k_n (up to $n = 20$, say) can be obtained, by (28), from coefficients $\bar{a}_{nm}$ and $\bar{b}_{nm}$ determined by a combination of satellite and gravimetric data. Estimates from empirical gravity anomaly fields give certain 'local' parameters of the gravity anomaly covariance function.

It has turned out that the gravity anomaly covariance function $C(\psi)$, the function (30) restricted to the sphere $r = R$, can be characterized, to an accuracy that is sufficient for many applications, by three 'essential' parameters (Figure 2):

Variance

$$C_0 = C(0) = \text{var}(\Delta g) \tag{32}$$

Correlation length ξ defined by

$$C(\xi) = \tfrac{1}{2}C_0 \tag{33}$$

Gradient variance

$$G_0 = \text{var}(\partial\Delta g/\partial s) \tag{34}$$

$\partial\Delta g/\partial s$ denoting the gradient of Δg along a horizontal direction; also,

$$G_0 = \tfrac{1}{2}\,\text{var}(\partial\Delta g/\partial h) \tag{35}$$

where $\partial\Delta g/\partial h$ denotes the vertical gradient of Δg. The parameter G_0 equals the curvature κ of the curve $C(\psi)$ at $\psi = 0$:

$$\kappa = 1/\rho = G_0 \tag{36}$$

[cf. *Moritz*, 1976*b*, section 3].

A good estimate for the global variance C_0 of the gravity anomaly is [*Tscherning and Rapp*, 1974, p. 20]

$$C_0 = 1795 \text{ mGal}^2 \tag{37}$$

The other two local parameters are far less reliable; one might take

Correlation length

$$\xi = 70 \text{ km} \tag{38a}$$

Gradient variance

$$G_0 = 2 \text{ mGal}^2 \text{ km}^{-2} \tag{38b}$$

Tscherning and Rapp [1974] have modeled the general trend of the lower degree variances c_3 to c_{20}, as well as C_0, by means of the expression

$$C(P, Q) = \alpha \sum_{n=3}^{\infty} \frac{n-1}{(n-2)(n+B)} \sigma^{n+2} \cdot \left(\frac{R^2}{r_P r_Q}\right)^{n+2} P_n(\cos\psi) \tag{39}$$

which contains the three free parameters α, B, and σ. If in addition to the lower degree variances and to C_0, one wishes to model also the local characteristics G_0 and ξ, one may use a model

$$C(P, Q) = \alpha_1 \sum_{3}^{\infty} \frac{n-1}{n+A} \sigma_1^{n+2} \left(\frac{R^2}{r_P r_Q}\right)^{n+2} P_n(\cos\psi) + \alpha_2 \sum_{3}^{\infty} \frac{n-1}{(n-2)(n+B)} \sigma_2^{n+2} \left(\frac{R^2}{r_P r_Q}\right)^{n+2} P_n(\cos\psi) \tag{40}$$

which contains six parameters, α_1, α_2, A, B, σ_1, and σ_2 [*Moritz*, 1977].

The only global empirical point anomaly covariance function available so far seems still to be *Kaula*'s [1959] determination; the model by *Tscherning and Rapp* [1974] has been derived from 1° × 1° mean anomalies together with a point variance C_0. A new reliable determination of a worldwide covariance function that represents both global and local features is highly desirable.

Plane covariance models. For certain limited purposes, such as interpolation, one may approximate the terrestrial sphere locally by a plane. Let (x, y) denote rectangular coordinates in the plane, and let the points $P(x_P, y_P)$ and $Q(x_Q, y_Q)$ be restricted to the plane. Then homogeneity and isotropy imply that the covariance function (say, of Δg) can depend only on the plane distance $s = PQ$, given by

$$s^2 = (x_P - x_Q)^2 + (y_P - y_Q)^2 \tag{41}$$

Possible analytical expressions (they must be positive definite) are, for instance,

$$C(s) = C_0 e^{-A^2 s^2} \tag{42}$$

$$C(s) = C_0/(1 + B^2 s^2)^m \tag{43}$$

with the suitable constants A, B, C_0, and m. An example is Hirvonen's regional covariance function for Ohio, which is (43) with $C_0 = 337 \text{ mGal}^2$, $B^{-1} = 40$ km, and $m = 1$ [*Heiskanen and Moritz*, 1967, p. 255].

If the points P and Q are no longer restricted to the xy plane but may lie in the upper half space (the space above the xy plane), then the spatial covariance function must be harmonic as a function of both (x_P, y_P, z_P) and (x_Q, y_Q, z_Q), the z axis being, of course, normal to the xy plane and positive upward. The model (42) cannot easily be extended into the upper half space so as to obtain a harmonic function. For the model (43) this is possible for $m = \frac{1}{2}$ and $m = \frac{3}{2}$:

$$C(P, Q) = \frac{C_0 b}{[s^2 + (z_P + z_Q + b)^2]^{1/2}} \tag{44}$$

and

$$C(P, Q) = \frac{C_0 b^2 (z_A + z_B + b)}{[s^2 + (z_P + z_Q + b)^2]^{3/2}} \tag{45}$$

respectively. Here, b is a constant, and s is again given by (41). For $z_A = z_B = 0$ the functions (44) and (45) reduce to (43), with $B = b^{-1}$ [cf. *Moritz*, 1976*b*, pp. 41–42].

Other possible plane covariance functions are derived from the Markov model:

$$C(s) = C_0 e^{-s/D} \tag{46}$$

They are called higher-order Markov models:

$$C(s) = C_0[1 + (s/D)]e^{-s/D} \tag{47}$$

$$C(s) = C_0[1 + (s/D) + (s^2/3D^2)]e^{-s/D} \tag{48}$$

For discussions and uses of them, see *Jordan* [1972], *Kasper* [1971], and *Shaw et al.* [1969].

Empirically, values of the covariance functions can be determined by suitable sampling methods. A simple procedure is as follows. Cover the plane region under consideration by a square grid of width a, and assume the region itself to be a rectangle of sides Ma and Na, M and N being integers. Then the values of Δg at the grid points form a rectangular matrix $\Delta g_{i,j}$, where $i = 1, 2, \cdots, M$ and $j = 1, 2, \cdots, N$. We get 'north-south' covariances

$$C'(ka) = \frac{1}{(M-k)N} \sum_{j=1}^{N} \left(\sum_{i=k+1}^{M} \Delta g_{i-k,j} \Delta g_{i,j} \right) \tag{49a}$$

and 'east-west' covariances

$$C''(ka) = \frac{1}{M(N-k)} \sum_{i=1}^{M} \left(\sum_{j=k+1}^{N} \Delta g_{i,j-k} \Delta g_{i,j} \right) \tag{49b}$$

the weighted mean of which forms the desired estimates:

$$C(ka) = \frac{(M-k)NC'(ka) + M(N-k)C''(ka)}{(M-k)N + M(N-k)} \tag{50}$$

Thus we obtain estimates for the covariance function $C(s)$ for $s = 0, a, 2a, 3a, \cdots$, and we can try to fit an analytical expression to these discrete values. A Fortran program for covariance computation is given by *Rapp* [1966].

Nonisotropy. So far, we have assumed the covariance functions for T and Δg to be isotropic, that is, independent of azimuth. Such functions have been used almost exclusively so far. Nonisotropic covariance functions have been studied by several authors [cf. *Grafarend*, 1976; *Morrison*, 1977; *Rummel and Schwarz*, 1977].

Various other aspects of covariance functions are discussed by *Bellaire* [1977], *Groten* [1970], *Kubackova* [1974, 1976], *Meissl* [1971], *Tscherning* [1973, 1976], and *Vyskocil* [1970].

4. CONSIDERATION OF RANDOM ERRORS AND SYSTEMATIC PARAMETERS

Collocation with random errors. The collocation formula (22) is valid if the observed 'functionals' l_i are errorless. Frequently, however, random measuring errors n_i (the 'noise') must be taken into account, so we now have

$$l_i = s_i + n_i \tag{51}$$

where s_i (the 'signal') denotes the errorless part of l_i and represents the purely gravitational effect (e.g., errorless gravity anomalies or deflections of the vertical).

Let $[C_{ij}]$ denote, as before, the signal covariance matrix:

$$C_{ij} = M\{s_i s_j\} \tag{52}$$

to be derived from the covariance function (section 3) by 'covariance propagation' according to (20). Let, similarly, $[D_{ij}]$ denote the error covariance matrix, which is the variance-covariance matrix of the measuring errors n_i (only this matrix is considered in usual least-squares adjustment). Then the matrix

$$[\bar{C}_{ij}] = [C_{ij} + D_{ij}] \tag{53}$$

represents the total covariance matrix of the vector of observed functionals l_i.

It is now quite remarkable that the only modification of (22) to take measuring errors into account is the replacement of the matrix $[C_{ij}]$ by the total covariance matrix $[\bar{C}_{ij}]$ as given by (53); the covariances C_{Pk} remain unchanged.

We can also easily free ourselves from the requirement that the function $f(P)$ to be estimated is the anomalous potential. In fact, we can use (22), or its modification for random errors just mentioned, for the estimation of any quantity of the anomalous gravity field such as gravity anomalies, geoidal height, deflections of the vertical, spherical harmonic coefficients, etc. All such quantities s are linear functionals of T; symbolically,

$$s = L^P T(P) \tag{54}$$

Applying the linear functional L^P to both sides of (22), we see that $f(P)$ is replaced by the signal $\hat{s}$ to be estimated and C_{Pk} must be replaced by

$$C_{sk} = L^P C_{Pk} = L^P L_k{}^Q K(P, Q) \tag{55}$$

everything else remaining unchanged.

Together with the introduction of $\bar{C}_{ij}$ instead of C_{ij} this gives finally

$$\hat{s} = [C_{s1}\, C_{s2} \cdots C_{sq}] \begin{bmatrix} \bar{C}_{11} & \bar{C}_{12} & \cdots & \bar{C}_{1q} \\ \bar{C}_{21} & \bar{C}_{22} & \cdots & \bar{C}_{2q} \\ \vdots & \vdots & & \vdots \\ \bar{C}_{q1} & \bar{C}_{q2} & \cdots & \bar{C}_{qq} \end{bmatrix}^{-1} \begin{bmatrix} l_1 \\ l_2 \\ \vdots \\ l_q \end{bmatrix} \tag{56}$$

In abbreviated matrix form this may be written

$$\hat{s} = \mathbf{C}_{sl}\bar{\mathbf{C}}_{ll}{}^{-1}\mathbf{l} \tag{57}$$

which again has the form of the Wiener-Kolmogorov prediction formula but applied to heterogeneous quantities. In this form the simple prediction formula is really quite universal.

Let us mention some of its properties. The formula (57) again minimizes the estimation error of s; it provides a best linear estimate in the statistical sense: an unbiased linear estimate of minimum variance. Clearly, (56) represents a linear combination of signal covariances

$$\hat{s} = \sum_{k=1}^{q} b_k C_{sk} \tag{58}$$

It is immediately seen that measuring errors do not affect the C_{sk}, which are purely analytical; the statistics of measuring errors influences only the 'best' estimation of the coefficients b_k in the sense just mentioned.

There is thus a 'clean' mathematical model at the base of the collocation formula (56), represented by the analytical character of the covariance function $K(P, Q)$ and of the signal covariances C_{ij}, C_{Pk}, and C_{sk} derived from it by the 'covariance propagation' formulas (20), (21), and (55); the latter are now seen to carry the precise functional structure of the terrestrial gravitational field.

Let us briefly compare the present model and 'errorless' or 'exact' collocation as described in section 2. Both models are formally identical; they differ, however, in the underlying mechanism. In exact collocation the kernel function $K(P, Q)$ may be taken as a covariance function to obtain a statistically best estimate, or the kernel function may be selected freely to possess certain desirable analytical characteristics such as simplicity; in either case the q coefficients b_k are completely determined by the condition that the interpolation function exactly fits q given functionals. In collocation with noise the kernel function $K(P, Q)$ may again be taken as a covariance function of the anomalous gravity field; the coefficients b_k are now determined in such a way that the effect of random measuring errors in the given functionals is filtered out as much as possible: the functionals are no longer exactly reproduced.

Since the basic work by *Krarup* [1969], such collocation models have been widely applied for estimating the geoid by a combination of various data and for other purposes [cf. *Grafarend,* 1971; *Grafarend and Offermanns,* 1975; *Heitz and Tscherning,* 1972; *Lachapelle,* 1975; *Moritz,* 1970; *Rapp,* 1973, 1974, 1975; *Tscherning,* 1975*b*; *Zieliński,* 1975].

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

We shall therefore consider observations x_i that include a 'systematic' part besides the 'random' part (51):

$$x_i = \sum_{r=1}^{m} A_{ir}X_r + s_i + n_i \qquad i = 1, 2, \cdots, q \tag{59}$$

or, in matrix notation,

$$\mathbf{x} = \mathbf{AX} + \mathbf{s} + \mathbf{n} \tag{60}$$

The vector $\mathbf{x}$ comprises the q measured quantities, and $\mathbf{s}$ and $\mathbf{n}$ are the signal and noise parts as in (51). The new component is $\mathbf{AX}$, where the vector $\mathbf{X}$ comprises m systematic nonrandom parameters and $\mathbf{A}$ is a known $q \times m$ matrix, $m < q$. In general, the linear relation $\mathbf{AX}$ will be a linearization of an originally nonlinear function.

This model is generally enough to encompass all conceivable geodetic measurements. In fact, any geodetic measurement can be split into three parts, corresponding to (60): (1) a systematic part $\mathbf{AX}$ involving, on the one hand, the ellipsoidal reference system and, on the other hand, other parameters and systematic errors, (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, depending on the parameters of the reference ellipsoid, as well as systematic errors such as gravimeter drift; $\mathbf{s}$ is the gravity anomaly Δg; and $\mathbf{n}$ stands for the measuring error [cf. *Moritz*, 1969].

In this case the best linear estimate is

$$\hat{\mathbf{X}} = (\mathbf{A}^T\mathbf{C}_{xx}^{-1}\mathbf{A})^{-1}\mathbf{A}^T\mathbf{C}_{xx}^{-1}\mathbf{x} \tag{61}$$

$$\hat{\mathbf{s}} = \mathbf{C}_{sx}\mathbf{C}_{xx}^{-1}(\mathbf{x} - \mathbf{A}\hat{\mathbf{X}}) \tag{62}$$

where $\mathbf{C}_{xx}$ is the matrix (53):

$$\mathbf{C}_{xx} = \mathbf{C}_{ll} = \bar{\mathbf{C}} = [C_{ij} + D_{ij}] \tag{63}$$

Equation (61) is analogous to classical least-squares adjustment by parameters [cf. *Bjerhammar*, 1973, p. 123] except that now the covariance matrix $\mathbf{C}_{xx}$ includes the covariances of the signal as well as those of the measuring errors. Equation (62) is an obvious generalization of (57) to the case in which the average of $\mathbf{x}$ is no longer zero but $\mathbf{AX}$. The vector $\hat{\mathbf{s}}$ comprises one or several estimated signals $\hat{s}_\alpha$ ($\alpha = 1, 2, \cdots, p$); consequently, $\mathbf{C}_{sx}$ is a $p \times q$ matrix consisting of p rows of the form $[C_{s1}, C_{s2}, \cdots, C_{sq}]$ as entering in (56). The estimated $\hat{s}_\alpha$ can be completely different from the s_i in (59), or they can also be estimates for them.

These formulas are an extension of the corresponding problem for time series [*Grenander and Rosenblatt*, 1957, p. 87]. Similar models have already been used by *Kaula* [1963].

The estimates (61) and (62), like all least-squares estimates, satisfy two different minimum principles: (1) least variances of the estimated quantities $\hat{\mathbf{X}}$ and $\hat{\mathbf{s}}$, which thus represent statistically best estimates, and (2) a minimum condition

$$\mathbf{v}^T\mathbf{K}^{-1}\mathbf{v} = \min \tag{64}$$

where the $p + q$ vector $\mathbf{v}$ consists of the p estimated signals $\hat{s}_\alpha$ and the q measuring errors n_i (or rather their estimates $\hat{n}_i$) and $\mathbf{K}$ is the covariance matrix of $\mathbf{v}$.

The present model may be regarded as a combination of least-squares adjustment and least-squares prediction into a unified scheme. It provides a comprehensive method for an optimal combination of all geodetic data—classical angle and distance measurements, astronomical observations, gravity measurements, satellite data of different kinds, etc.—to obtain the geometric position of points on the earth's surface as well as the gravitational field. In practice, the amount of data that can be combined is limited by the size of the matrix that can be inverted on the computer. This requires suitable representative selection of the data and some working 'from the large to the small' in several steps.

Accuracy. The variance-covariance matrices $\mathbf{E}_{XX}$ and $\mathbf{E}_{ss}$ describing the accuracy of the estimates $\hat{\mathbf{X}}$ and $\hat{\mathbf{s}}$ are given by

$$\mathbf{E}_{XX} = (\mathbf{A}^T\mathbf{C}_{xx}^{-1}\mathbf{A})^{-1} \tag{65}$$

$$\mathbf{E}_{ss} = \mathbf{C}_{ss} - \mathbf{C}_{sx}\,\mathbf{C}_{xx}^{-1}\,\mathbf{C}_{sx}^T + \mathbf{C}_{sx}\,\mathbf{C}_{xx}^{-1}\mathbf{A}\mathbf{E}_{XX}\,\mathbf{A}^T\mathbf{C}_{xx}^{-1}\mathbf{C}_{sx}^T \tag{66}$$

The matrix $\mathbf{C}_{ss}$ represents the signal covariance matrix for the vector $\hat{\mathbf{s}} = [\hat{s}_\alpha]$. If the true values s_α of the estimates $\hat{s}_\alpha$ are given by

$$s_\alpha = L_\alpha^P T(P) \tag{67}$$

then the elements $C_{\alpha\beta}$ of the matrix $\mathbf{C}_{ss}$ are given by

$$C_{\alpha\beta} = L_\alpha^P L_\beta^Q K(P, Q) \tag{68}$$

in analogy to (20).

A derivation of these formulas is given by *Moritz* [1973, section 3]. In addition to their use in estimating the accuracy of computed quantities, they may also be applied for feasibility studies such as the planning of surveys. They do not require actual data, but they presuppose good estimates of the covariances involved. Applications have been made, for instance, to the planning of gravity surveys [*Tscherning*, 1975*a*] and to feasibility studies involving aerial gradiometry [*Schwarz*, 1976*b*, 1977] and satellite gradiometry [*Kryński et al.*, 1977]. Literature on the relation between least-squares adjustment and collocation includes papers by *Blaha* [1976], *Koch* [1977], *Rummel* [1976], *Schwarz* [1976*a*], and *Wolf* [1974]. Collocation methods have been applied in photogrammetry [*Kraus and Mikhail*, 1972], in meteorology [*Baussus von Luetzow*, 1973], and in other fields. Related methods have been discussed, among others, by *Bjerhammar* [1975*a*, *b*, 1976], *Groten* [1973, 1974], *Monget and Albuisson* [1971], and *Thomas and Heller* [1976]. Relations between collocation and geodetic boundary value problems have been investigated by *Krarup* [1969], *Bjerhammar* [1975*a*, 1976], *Moritz* [1976*a*], and *Neyman* [1974, 1975, 1977]. A very general Fortran program for applications of collocation has been given by *Tscherning* [1974].

5. RELATION TO GEOPHYSICAL INVERSE PROBLEMS

A complete mathematical description of the irregular gravitational field inevitably involves infinitely many parameters, for instance, the set of all coefficients in the spherical harmonic expansion of the disturbing potential T; let us arrange these coefficients into an infinite sequence

$$s_1, s_2, s_3, \cdots \tag{69}$$

Since they refer to the anomalous gravity field, the 'signal field,' they themselves have the character of signals.

Every quantity l_i of the anomalous gravity field can be expanded into a series of spherical harmonics provided this series converges:

$$l_i = \sum_{r=1}^{\infty} b_{ir}s_r \tag{70}$$

Let us again have q observations, so that $i = 1, 2, \cdots, q$. Each observation l_i may be expanded in the form (70). We thus have a system of q linear equations for infinitely many unknowns. This is clearly an underdetermined problem: There are infinitely many possible sets of solutions.

A unique best (in the statistical sense outlined above) linear solution is provided by least-squares collocation. On admitting measuring errors n_i the system (70) is replaced by

$$\sum_{r=1}^{\infty} b_{ir}s_r + n_i = l_i \qquad i = 1, 2, \cdots, q \tag{71}$$

or, in matrix symbolism,

$$\mathbf{Bs} + \mathbf{n} = \mathbf{l} \tag{72}$$

$\mathbf{B}$ being a matrix with q rows and infinitely many columns. Denote the signal covariance matrix of the infinite vector $\mathbf{s}$ by $\mathbf{K}$; this matrix is found to be an infinite diagonal matrix whose diagonal elements are proportional to the k_n in (29). Let the covariance matrix of the measuring errors be denoted by $\mathbf{D}$, and let $\mathbf{s}$ and $\mathbf{n}$ be uncorrelated, as usual. Then the application of covariance propagation to (72) gives readily

$$\mathbf{C}_{ll} = \mathbf{BKB}^T + \mathbf{D} \tag{73}$$

$$\mathbf{C}_{sl} = \mathbf{KB}^T \tag{74}$$

for the autocovariance matrix $\mathbf{C}_{ll}$ of $\mathbf{l}$ and the cross-covariance matrix $\mathbf{C}_{sl}$ between $\mathbf{s}$ and $\mathbf{l}$. Then (57) gives for the estimate $\hat{\mathbf{s}}$ of the spherical harmonic coefficient vector $\mathbf{s}$

$$\hat{\mathbf{s}} = \mathbf{K}\mathbf{B}^T(\mathbf{B}\mathbf{K}\mathbf{B}^T + \mathbf{D})^{-1}\mathbf{l} \tag{75}$$

For $\mathbf{D} = 0$ we get the usual solution of the errorless equation (70) with $\mathbf{n} = 0$ by means of generalized inverses, $\mathbf{K}\mathbf{B}^T(\mathbf{B}\mathbf{K}\mathbf{B}^T)^{-1}$ being a generalized inverse of $\mathbf{B}$ and different $\mathbf{K}$ corresponding to different inverses.

The mathematical model (70) or (72) and the solution (75) have also been suggested for geophysical inverse problems [cf. *Burkhard and Jackson*, 1976; *Wiggins*, 1972, pp. 260–261]. In fact, the determination of the earth's external gravity field from observations also has the character of an underdetermined 'improperly posed' problem: the finite number of observations can never fully determine the infinite number of parameters of the gravity field. Here we mention also the Hilbert space approach of *Backus* [1970].

The solution (75) has favorable numerical properties, especially stability. In the case of the terrestrial gravity field the covariance matrices $\mathbf{K}$ and $\mathbf{D}$ are not just auxiliary mathematical quantities introduced to obtain a convenient solution; they admit of a physical definition in terms of the statistics of the anomalous gravitational field and are, in principle, determinable by observation.

The accuracy of the estimated spherical harmonic coefficients can be estimated by (66) with $\mathbf{A} = 0$ and $\mathbf{C}_{ss} = \mathbf{K}$. If $\mathbf{E}_{ss}$ and $\mathbf{C}_{ss}$ are simultaneously transformed into diagonal form, then the comparison of the respective diagonal terms provides an objective criterion on whether a certain coefficient s_r can be meaningfully determined from the data or not.

The present model has been applied to the determination of zonal and, in part, also tesseral harmonics by *Balmino et al.* [1976], *Moritz and Schwarz* [1973], *Reigber and Ilk* [1976], and *Schwarz* [1974, 1975*a*, *b*].

6. ANALYTICAL AND STATISTICAL ASPECTS

Least-squares collocation has its roots in many fields: (1) least-squares estimation, (2) stochastic processes and spectral analysis, (3) approximation theory, (4) functional analysis, especially the theory of Hilbert spaces with kernel functions, (5) potential theory, and (6) inverse and improperly posed problems. These fields are frequently overlapping but sufficiently characteristic to be mentioned. All of these 'many facets of collocation' must be taken into consideration if a one-sided treatment is to be avoided.

Most obvious is the relation to classical least-squares estimation. In fact, collocation models bear resemblance to conventional adjustment models. The geometrical interpretation in terms of simple geometrical operations, projection on subspaces, is similar. Similar too is the invariance with respect to linear transformations, which is fundamental, since it ensures consistency: whichever quantity we compute by collocation, it always refers to the same gravity field. The characteristic difference is the infinite number of spectral parameters necessary to characterize the gravitational field fully. Hence one must operate in an infinite-dimensional Hilbert space rather than in finite linear spaces; this is a subtle but essential difference. It is here that the theory of stochastic processes and their spectral analysis by a spherical harmonic representation enters.

Least-squares estimation and stochastic processes provide a very convenient mathematical formalism and terminology and also a statistical interpretation of the results. However, this statistical interpretation may sometimes have been too much in the foreground and may have hidden the equally significant analytical aspects of collocation. Therefore we have attempted here to approach collocation from the point of view of approximation theory, working with a kernel function $K(P, Q)$ which can, in principle, be arbitrary; we take $K(P, Q)$ to be a statistically defined covariance function only to get a best estimate. However, as we have said, it is fully legitimate to take for $K(P, Q)$ any positive definite harmonic function; then collocation may be regarded as a purely analytic interpolation in a Hilbert space with a kernel function, even without stochastic interpretation. (There is also a relation between stochastic processes and kernel functions which dates back to *Parzen* [1961].) In fact, how seriously the statistical interpretation is taken is a matter of controversy and also of personal taste. Formulas such as (61) and (62) remain the same; only the interpretation of the estimated variances and covariances (65) and (66) and the best character of the estimates depend on statistics.

It is tempting to consider the anomalous gravity field as a stochastic process on a sphere. The main argument in favor of such an interpretation, as we have mentioned, is the obvious interpretation of covariances, prediction formulas, etc., in terms of stochastic process theory. There are, however, two counterarguments. First, there is only one earth; a probability space of possible earths may appear physically unnatural, although it is logically unobjectionable. Second, *Lauritzen* [1973] has proved that it is impossible to find a stochastic process harmonic outside the sphere that is both Gaussian and ergodic. This does not preclude non-Gaussian ergodic processes but may enhance the argument of unnaturality. Therefore it has been proposed that the stochastic process interpretation be dropped in favor of an interpretation in terms of Wiener's 'covariance analysis of individual functions' [cf. *Doob*, 1949, section 1], interpreting the averaging operator M not as a stochastic expectation (average over a probability space of many functions) but as the average of one function over rotation group space (24), that is, over the whole earth and over all directions. This allows the statistical interpretation of the variances of estimated quantities as average accuracies over an area. Observation errors, which do have a probability distribution and a stochastic expectation E, are readily incorporated by regarding as the total averaging operator the commutative product $EM = ME$ [*Moritz*, 1973, sections 8 and 9]. More about analytical and stochastic aspects of collocation is given by *Dermanis* [1976], *Eeg and Krarup* [1975], and *Tscherning* [1977].

It should be pointed out that the non-Gaussian character of the anomalous gravitational field implies that the 'best linear' estimate is not the absolutely best estimate: nonlinear estimates may still reduce the variance of the result. Therefore nonlinear prediction has been suggested, among others, by *Grafarend* [1972] and *Kaula* [1966].

Potential theory enters most obviously, but relatively superficially, through the harmonic character of the spatial covariance function. Subtler but perhaps even more important is the fact that the physical structure of the anomalous gravitational field with its precise mathematical relations between its quantities—T, Δg, ξ, η, and N—is reflected in linear operations on the analytical base functions $\phi_k(P)$. The statistical interpretation of these operations as 'covariance propagation' should not veil the fact that they are essentially analytical.

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(Received December 8, 1977;
accepted March 16, 1978.)