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A NOTE ON THE CHOICE OF NORM WHEN USING COLLOCATION FOR THE COMPUTATION OF APPROXIMATIONS TO THE ANOMALOUS POTENTIAL

Abstract

In order to use the method of (least squares) collocation for the computation of an approximation to the anomalous potential of the Earth (T) it is necessary to specify a reproducing kernel Hilbert space the dual of which contain the (linear) functionals associated with the observations.

The specification includes the prescription of an inner product or an equivalent norm. It is demonstrated, that this is equivalent to the prescription of a specific reproducing kernel when an orthogonal (but not necessarily orthonormal), countable basis is known.

When T is an element of the Hilbert space, it is proved, that absolute error bounds may be computed, provided the norm of T is known. Also the convergence of a sequence of approximations obtained using observations increasing in a regular fashion is secured in this case as proved by Moritz.

In Geodetic practice the empirical covariance function of the anomalous potential has been used as a reproducing kernel and has in connection with the set of solid spherical harmonics specified a norm. It is proved, that a Hilbert space (of infinite dimension) equipped with this norm does not contain the anomalous potential.

1. Introduction

The gravity potential of the Earth (W) is the sum of a gravitational potential and a rotational potential. Let us suppose, that we have adopted a certain reference potential (U) which rotational part is exactly equal to the rotational part of W and which contains the influence of the atmosphere. The difference $T = W - U$ is then denoted the anomalous potential and will be a harmonic function outside the masses of the Earth.

We will throughout this paper work is ***spherical approximation*** (see e.g. Moritz (1976, p. 2) for a definition of this term). The Earth is then approximated by a sphere with radius $R = 6371$ km . Outside this sphere we may expand T in normalized solid spherical harmonics (see Heiskanen and Moritz (1967, eq. (1–77a and 1–77b)).). For a point P with spherical coordinates (φ, λ, r) (latitude, longitude and distance from the origin) we have

$$T(P) = \frac{kM}{r} \sum_{i=2}^{\infty} \left(\frac{R}{r}\right)^i \sum_{i=0}^{i} \bar{P}_{ij}(\sin\varphi)\left[\bar{C}_{ij}\cos(j\lambda) + \bar{S}_{ij}\sin(j\lambda)\right] \quad (1)$$

Bull. Geod. 51 (1977) pp. 137–147.

where k is the gravitational constant, M is the mass of the Earth, $\bar{C}_{ij}$ and $\bar{S}_{ij}$ are the (unitless) coefficients of the series and $\bar{P}_{ij}$ are the normalized associated Legendre polynomials.

It will frequently be necessarily to deal with two points P, Q in space. The spherical coordinates of Q will be denoted φ', λ' and r' and correspondingly will quantities (functions or functions of functions, so–called functionals) evaluated at or related to Q carry an apostrophe. With this convention we have for example $T(P) = T$, $T(Q) = T'$ and $\Delta g(Q) = \Delta g' = L'_{\Delta g}(T)$ where $L'_{\Delta g}$ is the functional which to an arbitrary T associates its gravity anomaly in the point Q.

The method of least squares collocation may be used for the computation of an approximation to the anomalous potential. Given a set of n observed quantities $\{m_i\}$; where $i = 1, \ldots, n$, related to T by a *linear* functional L_i, i.e.

$$L_i(T) = m_i, \qquad i = 1, \ldots, n \tag{2}$$

it is possible to find an approximation $\tilde{T}$ to T which agrees with the observed quantities (i.e. eq. (2) is valid for $\tilde{T}$) and which has the least norm, provided the linear functionals L_i are elements of the space dual to a reproducing kernel Hilbert space. (See Davis (1975) or Meissl (1975, 1976) for an introduction to reproducing kernel Hilbert spaces).

Let us denote the space H and the dual space H'. (The dual space consists of the continuous, linear mappings from H to the real numbers, i.e. the linear functionals). H is specified by its elements (which here will be a subset of the harmonic functions), and its inner product or corresponding norm. The inner product of two elements of H, f and g is denoted (f, g) and the norm $\|f\|$, where $\|f\|^2 = (f, f)$.

Example :

The functions harmonic outside the sphere with radius R having square integrable boundary values. An inner product is then (σ is the surface of the sphere)

$$(f, g) = \frac{1}{4\pi} \int_\sigma f \cdot g \, d\sigma , \tag{3}$$

with corresponding norm

$$\|f\|^2 = \frac{1}{4\pi} \int_\sigma f^2 \, d\sigma , \tag{4}$$

where the integral must be interpreted as the limit of the integrals over concentric spheres having radii $R + \epsilon$, $\epsilon \to 0$, $\epsilon > 0$.

In section 2 the relationship between the norm and the reproducing kernel in a separable Hilbert space is used to prove that the choice of a specific function as a reproducing kernel will determine the norm when an orthogonal base is known.

The role and choice of norm in connection with the application of collocation is discussed in section 3 and 4. In section 3 it is proved, that when the norm is chosen so that T is an element of the Hilbert space, it will be possible to obtain absolute error estimates for $\tilde{T}$ provided the norm of T is known.

In section 5 it is proved, using the results of section 2, that T is not an element of the Hilbert space implicitly specified by choosing the so-called empirical covariance function to be the reproducing kernel of the space. Some consequences of this are discussed in the final section 6.

2. The Relationship Between Norm and Reproducing Kernel in a Separable Hilbert Space.

A separable Hilbert space is a Hilbert space in which there exist an orthonormal base consisting of a countable number of elements of the space. When Hilbert spaces of harmonic functions have a reproducing kernel they will be separable, cf. e.g. Meschkowski (1963, Theorem III 8). In the following we will therefore suppose that we are dealing with separable Hilbert spaces. Let us denote the elements of the base by the doubly subscripted quantities (functions) V_{ij}, $i = 1, \ldots, \infty$, $-i \leqslant j \leqslant i$, i.e.

$$\| V_{ij} \| = 1$$

and

$$(V_{ij}, V_{nm}) = \begin{cases} 1 \text{ for } i = n \text{ and } j = m \\ 0 \text{ for } i \neq n \text{ or } j \neq m . \end{cases} \tag{5}$$

Any element of the space can be expanded in an infinite series (with coefficients a_{ij})

$$f(P) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} a_{ij} V_{ij}(P) , \tag{6}$$

and we have

$$\|f\|^2 = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} a_{ij}^2 < \infty \tag{7}$$

The reproducing kernel is then (cf, e.g. Meissl (1976, theorem 11.3 (2)))

$$K(P, Q) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} V_{ij}(P) \cdot V_{ij}(Q) . \tag{8}$$

Given an *orthogonal* base with elements denoted V_{ij}^*, where $\| V_{ij}^* \| = v_{ij}$, an *orthonormal* base is simply obtained by defining

$$V_{ij}(P) = \frac{1}{v_{ii}} V_{ij}^*(P) \tag{9}$$

and we have

$$K(P, Q) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} (v_{ij})^{-2} V_{ij}^*(P) V_{ij}^*(Q) . \tag{10}$$

Example (continued) : Let us put

$$V^*_{ij}(P) = \frac{1}{r}\left(\frac{R}{r}\right)^i \bar{P}_{ij}(\sin\varphi) \cdot \begin{cases} \cos(j\lambda), & j \geq 0 \\ \sin(j\lambda), & j < 0. \end{cases} \quad (11)$$

We then have using Heiskanen and Moritz (1967, eq. (1–74)),

$$\left\| V^*_{ij}(P) \right\|^2 = \frac{1}{4\pi} \int_\sigma (V^*_{ij}(P))^2 \, d\sigma = \frac{1}{R^2} \quad (12)$$

and thereby from eq. (10) and using Krarup (1969, eq. III (7))

$$K(P,Q) = \sum_{i=0}^{\infty} \sum_{j=0}^{i} \left(\frac{R^2}{r r'}\right)^{i+1} \bar{P}_{ij}(\sin\varphi) \bar{P}_{ij}(\sin\varphi') (\cos(j\lambda)\cos(j\lambda') + \sin(j\lambda)\sin(j\lambda'))$$

$$= \sum_{i=0}^{\infty} \left(\frac{R^2}{r r'}\right)^{i+1} (2i+1) P_i(\cos\psi) = R^2 ((r \cdot r')^2 - R^4)/\ell^3 \quad (13)$$

where ψ is the spherical distance between P and Q, P_i is the i'th Legendre – polynomial and $\ell = ((r r')^2 - 2R^2 r r' \cos\psi + R^4)^{\frac{1}{2}}$. It is then easily seen that the reproducing property

$$f(P) = (f(Q), K(P,Q)) = \frac{1}{4\pi} \int_\sigma f(Q) \cdot K(P,Q) \, d\sigma \quad (14)$$

is nothing but the validity of Poisson's integral equation for the sphere. Other examples of reproducing kernel Hilbert spaces can be found in Tscherning (1973).

Conversely, when knowing an orthogonal basis (V^*_{ij}) and the expansion of the reproducing kernel with respect to this basis the norm is determined :

For an arbitrary function we have

$$f(P) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} b_{ij} V^*_{ij}(P). \quad (15)$$

Then using eq. (9) we have

$$f(P) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} b_{ij} v_{ij} (v_{ij}^{-1} V^*_{ij}(P)) = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} (b_{ij} v_{ij}) V_{ij}(P) \quad (16)$$

and hence

$$\|f\|^2 = \sum_{i=0}^{\infty} \sum_{j=-i}^{i} (b_{ij} v_{ij})^2, \quad (17)$$

whereby the norm of any element of H is given.

3. The Role of the Norm in Collocation

Let us presuppose that a Hilbert space H with dual space H' and reproducing kernel $K(P,Q)$ is given so that $L_i \in H'$, $i = 1, \ldots n$, cf. eq. (2). Using collocation an approximation $\tilde{T} \in H$ to T can be found which fulfil eq. (2) and which has the least norm. This last requirement assures the uniqueness of $\tilde{T}$ when the linear functionals L_i of eq. (2) all are linear independent (considered as elements of the space H'). We have (cf. e.g. Tscherning (1975, section 2))

$$\tilde{T}(P) = \sum_{i=1}^{n} a_i L_i'(K(P,Q)) \qquad (18)$$

(L_i' is evaluated in Q), where

$$a_i = \{ L_i'(L_j(K(P,Q)))\}^{-1} \{ m_j \} , \quad i,j = 1, \ldots, n \qquad (19)$$

In the dual space H' the norm of an arbitrary element L is defined by

$$\|L\| = \max_{f \in h} \frac{|L(f)|}{\|f\|} . \qquad (20)$$

From this definition we get the important inequality

$$|L(f)| \leqslant \|f\| \cdot \|L\| . \qquad (21)$$

(Note, that in eq. (20) and (21) we do not use different symbols for the norm in H and in H'. Similary, we will not use different symbols for the inner products in H and H'. No confusion should be possible, because elements of H' throughout will be denoted by L or by L with a subscript, e.g. L_i).

The definition, eq. (20), implies that H and H' are isometrically isomorphic and it can be proved (see Davis (1975, Corollary 12.6.7)) that the inner product of two linear functionals L_i and L_j (evaluated in P, Q respectively) becomes

$$(L_i , L_j) = L_j' (L_i (K(P,Q))) . \qquad (22)$$

and hence

$$\|L\| = (L,L)^{\frac{1}{2}} = L'(L(K(P,Q))) . \qquad (23)$$

The condition that the linear functionals associated with the measurements (eq. (2)) are elements of H' is thereby seen to be equivalent to $\|L_i\| = L_i L_i'(K(P,Q)) < \infty$.

Let us now presuppose that T is an element of H, i.e. $\|T\| < \infty$. We are then able to compute an upper limit for the numerical difference between the "true" value $L(T)$ and a computed value $L(\tilde{T})$, where L is an arbitrary linear functional.

Using eq. (2), (18) and (19) we have

$$L(T) - L(\widetilde{T}) = L(T) - L\left(\sum_{i=1}^{n} a_i L_i' K(P,Q)\right)$$

$$= L(T) - \{LL_i' K(P,Q)\}^T \{L_i' L_j K(P,Q)\}^{-1} \{L_j(T)\}$$

$$= (L - \{LL_i' K(P,Q)\}^T \{L_i' L_j K(P,Q)\}^{-1} \{L_j\})T .$$

From eq. (21) and using the linearity of the inner product and the relation between the inner product and the norm (eq. (23)) we get

$$|L(T) - L(\widetilde{T})|$$

$$\leqslant \|T\| \cdot \| L - \{LL_i' K(P,Q)\}^T \{L_i' L_j K(P,Q)\}^{-1} \{L_j\} \|$$

$$= \|T\| \cdot [((L - \{LL_i' K(P,Q)\}^T \{L_i L_j K(P,Q)\}^{-1} \{L_j\}), (L - \{LL_k' K(P,Q)\}^T$$

$$\cdot \{L_k' L_m K(P,Q)\}^{-1} \{L_m\}))]^{\frac{1}{2}}$$

$$= \|T\| \cdot [(L,L) - 2\{LL_i' K(P,Q)\}^T \{L_i' L_j K(P,Q)\}^{-1} \{L' L_j K(P,Q)\}$$

$$+ \{LL_i' K(P,Q)\}^T \{L_i' L_j K(P,Q)\}^{-1} \{(L_j, L_m)\} \{L_k' L_m K(P,Q)\}^{-1} \{L' L_k K(P,Q)\}]^{\frac{1}{2}}$$

Using that $\{(L_j, L_m)\} = \{L_j L_m' K(P,Q)\}$ we finally have

$$|L(T) - L(\widetilde{T})|$$

$$\leqslant \|T\| \cdot [\|L\|^2 - \{LL_i' K(P,Q)\}^T \{L_i' L_j K(P,Q)\}^{-1} \{L' L_k K(P,Q)\}]^{\frac{1}{2}} . \quad (24)$$

Hence, absolute error bounds may be obtained provided $\|T\|$ is known.

(Note that for L equal to one of the functionals L_i the error bound is equal to zero. This is one of the important characteristics of collocation (applied using data considered errorless)).

The norm has then in this context three functions :

(a) it assures the uniqueness of the approximation $\widetilde{T}$,

(b) it defines the reproducing kernel and

(c) it makes available error estimates when $\|T\|$ is known and finite.

4. Choice of Norm when Applying Collocation for Approximation

The problem of choosing an appropriate norm has earlier been discussed in Tscherning (1975, 1975a), Sjöberg (1975) and the importance of the problem is stressed in Eeg and Krarup (1975, § 5).

The reason for choosing one norm instead of another must be because of the better or worse quality of the approximation $\widetilde{T}$ obtained.

Let us note that when an approximation $\tilde{T}$ has been determined, we may compute estimates of quantities $L(T)$ by simply evaluating $L(\tilde{T})$. (This was used in eq. (22)). A measure for the quality of a norm could then be the maximal numerical difference or the mean square variation of the difference between certain measured values not used for the computation of $\tilde{T}$ and the values obtained using $\tilde{T}$. Sjöberg (1975) has used this latter criterion for choosing an optimal reproducing kernel in between a given set of "reasonable" kernels.

In order to gain more insight into these types of criteria let us consider the following example. Imagine, that the gravity anomalies

$$L_{\Delta g}(T) = -\left.\frac{\partial T}{\partial r}\right|_P - \frac{2}{r}T(P) \tag{25}$$

in an area have a certain smooth variation, see Figure 1. Then we would naturally prefer, that the gravity anomalies computed by substituting $\tilde{T}$ for T in eq. (25) have a similar variation. Is it possible to use this requirement as a criterion for choosing the norm ?

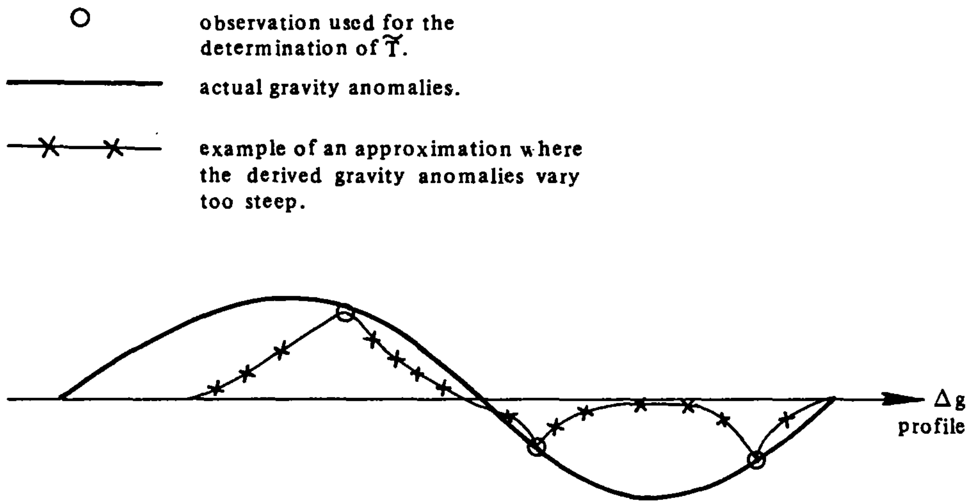

Fig. 1 – Gravity anomaly variation.

From eq. (24) we have

$$\left|\Delta g - L_{\Delta g}(\tilde{T})\right| \leq \|T\| \cdot \left(\|L_{\Delta g}\|^2 - \{L'_{\Delta g} L_i K(P,Q)\}^T \{L'_i L_j K(P,Q)\}^{-1} \{L'_j L_{\Delta g} K(P,Q)\}\right)^{\frac{1}{2}} \tag{26}$$

and by using eq. (21)

$$\left| L_{\Delta g} T \right| \leq \left\| T \right\| \cdot \left\| L_{\Delta g} \right\| . \tag{27}$$

Hence for $\| T \|$ we could choose

$$\| T \| \sim \frac{Max \left| L_{\Delta g} T \right|}{\| L_{\Delta g} \|}, \text{ (and } \| L_{\Delta g} \| \text{ equal to some constant)} \tag{28}$$

where the maximum is taken in the points of evaluation varying over the area of interest.

Consider then the situation where we only have one observation $L_0 T = M_0 = 0$ near this maximal value. The approximation $\tilde{T}$ given by eq. (18) would be identically zero and in the point where the maximal value occurred (P) we would have the error estimate (using eq. (26) and (28))

$$\begin{aligned} \left| L_{\Delta g}(T) - 0 \right| &\leq \| T \| \cdot \left(\| L_{\Delta g} \|^2 - (L_{\Delta g} L'_0 K(P,Q))^2 / (L'_0 L_0 K(P,Q)) \right)^{\frac{1}{2}} \\ &= \left((L_{\Delta g}(T))^2 - \| T \|^2 (L_{\Delta g} L'_0 K(P,Q))^2 / (L'_0 L_0 K(P,Q)) \right)^{\frac{1}{2}} . \end{aligned} \tag{29}$$

The inner product of the functionals L and L_0 must therefore be zero, otherwise the inequality will not hold.

In this way we could choose the inner product for a number of linear functionals – but it is obviously an impossible method and requires a perfect knowledge of T .

Instead of requiring the maximal error to be minimal one may require, that the mean square error is minimal when approximating T . But it can also be seen, that in order to fulfil this requirement a knowledge of T in all points is needed.

It is more realistic to require that the mean square error is minimized simultaneously for all configurations of measurements which after a rotation of the Earth become identical to the set given by eq. (2). As explained in Heiskanen and Moritz (1967, Chp. 7) an estimate of the mean frequency content of T per degree, the so–called degree–variances, are then needed. The reproducing kernel is in this case the (empirical) covariance function of the anomalous potential,

$$K(P,Q) = cov(T,T') = \sum_{i=2}^{\infty} \sigma_i(T,T) \left(\frac{R^2}{r r'}\right)^{i+1} P_i(\cos\psi) , \tag{30}$$

where

$$\sigma_i(T,T) = \left(\frac{kM}{R}\right)^2 \sum_{j=0}^{i} (\bar{C}_{ij}^2 + \bar{S}_{ij}^2) \tag{31}$$

are the (potential) degree–variances. (For a discussion of the actual estimation of $K(P,Q)$ see e.g. Tscherning and Rapp (1974)).

5. The Norm Determined by the Empirical Covariance Function

The reproducing kernel eq. (30) does only depend on the spherical distance between P and Q and the distances of P and Q from the origin. It is, cf. Lauritzen (1973, sections 7 and 8), "homogeneous with respect to the group of rotations around the origin". It must therefore be related to a norm which has the same property, i.e. a harmonic function is after a rotation of its domain of definition mapped in a harmonic function with the same norm.

For such a norm we know an orthogonal base, namely the solid spherical harmonics given by eq. (11). Hence, according to section 2, the norm is given through the length (v_{ij}) of the elements of the base (V_{ij}^*) .

Let us suppose that $\sigma_i(T, T) > 0$ for all i . We then have, using eq. (11), (30) and Heiskanen and Moritz (1967, eq. (1–82′)) .

$$K(P,Q) = \sum_{i=2}^{\infty} \sum_{j=i}^{i} (\sigma_i(T,T)/(2i+1)) R^2 V_{ij}^*(P) \; V_{ij}^*(Q) \; . \qquad (32)$$

Using eq. (10) with $(v_{ij})^{-2} = (\sigma_i(T,T)/(2i+1)) R^2$ we see that the new orthonormal base is

$$V'_{ij}(P) = (\sigma_i(T,T)/(2i+1))^{\frac{1}{2}} R \cdot V_{ij}^*(P) \; . \qquad (33)$$

Then using eq. (1), (11) we see that T with respect to this base will have the expansion

$$T(P) = \sum_{i=2}^{\infty} [\sum_{j=0}^{i} kM \cdot \bar{C}_{ij} (\sigma_i(T,T)/(2i+1))^{-\frac{1}{2}} R^{-1} V'_{ij}(P)$$
$$+ \sum_{j=1}^{i} kM \, \bar{S}_{ij} (\sigma_i(T,T)/(2i+1))^{-\frac{1}{2}} R^{-1} V'_{i,-j}(P)] . \qquad (34)$$

The square of the norm of T is

$$\| T \|^2 = \sum_{i=2}^{\infty} \sum_{j=0}^{i} (kM)^2 (2i+1)/(\sigma_i(T,T) \cdot R^2) (\bar{C}_{ij}^2 + \bar{S}_{ij}^2)$$

and using eq. (31) we have

$$\| T \|^2 = \sum_{i=2}^{\infty} (2i+1) (\frac{kM}{R})^2 [\sum_{j=0}^{i} (\bar{C}_{ij}^2 + \bar{S}_{ij}^2)] \cdot [(\frac{kM}{R})^2 \sum_{j=0}^{i} (\bar{C}_{ij}^2 + \bar{S}_{ij}^2)]^{-1}$$
$$= \sum_{i=2}^{\infty} (2i+1) = \infty \; . \qquad (35)$$

Hence we have proved, that T is not an element of the Hilbert space with reproducing kernel equal to the covariance function of the anomalous potential, presupposing that an infinite number of the degree variances are different from zero, i.e. that the Hilbert space is infinite dimensional.

6. Conclusions

In section 5 we proved, that T is not an element of the Hilbert space most commonly used in Physical Geodesy for approximation or prediction purposes, when the expansion of T in solid spherical harmonics contained an infinite number of non–zero terms. Let us suppose that this is true and let us consider two consequences.

By inspecting eq. (24) we see that the maximal error bounds are not finite. Nevertheless, estimates of the mean square error can be obtained (see e.g. Heiskanen and Moritz (1967, eq. (7–64))). It is equal to the right hand side of eq. (24) with $\| T \| = 1$.

Moritz (1976, pp. 14–16) has proved, that a sequence of approximations $\tilde{T}_i$ computed by the method of collocation (eq. (18)) tend to T , when the number of observations increased in a regular fashion. In the proof was implicitly presupposed, that T was an element of the Hilbert space having the reproducing kernel equal to the one occurring in eq. (18). So convergence is not assured when the empirical covariance function (eq. (30)) is used. (Naturally, this does not imply that a proof for the convergence can not be found).

The use of the empirical covariance function as a reproducing kernel when applying collocation assures the best approximation in a least squares sense (cf. section 4). But it requires the estimation of the covariance function which in principle requires the complete knowledge of T , and the prediction errors have no upper bound.

But will the use of other types of norms give more satisfactory results ?

This question can not be answered at present. In addition, the choice of norm does also (as discussed in Tscherning (1975, section 3)) depend on other factors, e.g. the computational possibilities.

Acknowledgment

A first version of this paper was presented at the meeting on Mathematical Problems in Geodesy, Oberwolfach, FRG, April 1976 with the title "Choice of Norm in (Least Squares) Collocation".

Valuable suggestions by Dr. R. Rummel and Dr. P. Meissl are gratefully acknowledged.

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Received : 31.01.1977
Revised : 14.03.1977