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On the Convergence of Least Squares Collocation

C. C. TSCHERNING

Geodætisk Institut - Charlottenlund

Summary. — The method of (least squares) collocation may be used for the determination of an approximation to the anomalous potential of the Earth (T) which agrees with a finite set of observations. The method requires that the observations are related to T through linear functionals. These functionals must all be elements of the space dual to a reproducing kernel Hilbert space of harmonic functions, H.

Let the number of observations increase in a regular fashion, i.e. so that the associated linear functionals will span the dual space H'. Then it is shown that the corresponding sequence of approximations will converge *strongly* towards T provided T is an element of H.

Working in spherical approximation with rotational invariant norms it is shown that when using observed boundary values of T or of gravity anomalies, Δg, must T at least have first, respectively second order derivatives at the boundary which are square integrable in order to assure strong convergence.

SULLA CONVERGENZA DELLA COLLOCAZIONE PER MINIMI QUADRATI.

Sommario. — Il metodo della collocazione può essere usato per la determinazione di una approssimazione delle anomalie (T) del potenziale terrestre che soddisfa ad un insieme finito di osservazioni. Il metodo richiede che le osservazioni siano legate a T da funzionali lineari. Questi funzionali devono essere tutti elementi dello spazio duale ad uno spazio di Hilbert H di funzioni armoniche dotato di nucleo riproduttore.

Supposto che il numero di osservazioni aumenti in modo regolare, cioè tale che i funzionali lineari ad esse associati generino lo spazio duale H', si dimostra che la corrispondente sequenza di approssimazioni converge fortemente a T purché T sia un elemento di H.

Utilizzando l'approssimazione sferica con norme invarianti per rotazione, si dimostra che quando si usano i valori osservati sul contorno di T o delle anomalie di gravità Δg, T deve avere in superficie almeno derivate del primo e rispettivamente del secondo ordine, che siano a quadrato sommabile in modo da assicurare la convergenza in senso forte.

1. — INTRODUCTION

The anomalous potential of the Earth, T, is equal to the difference between the gravity potential (W) and a certain reference potential (U), i.e.

$$T = W - U \,. \tag{1}$$

We will presuppose that T is harmonic outside the masses of the Earth and fulfil the usual regularity conditions at infinity (implying e.g. no zero-order term in the spherical harmonic expansion).

Throughout this paper we will work in *spherical approximation*. The Earth is then approximated by a sphere with radius $R = 6371$ km. The surface of the sphere is denoted σ and the set outside the sphere Ω. In Ω we may expand T in normalized solid spherical harmonics $V^*_{ij}(P)$, $P \in \Omega$. For P having spherical coordinates (φ, λ, r) (latitude, longitude and distance from the origin) we have

$$V^*_{ij}(P) = \left(\frac{R}{r}\right)^{i+1} \bar{P}_{i|j|}(\sin\varphi) \begin{cases} \cos j\lambda & j \geq 0 \\ \sin |j|\lambda & j < 0 \,, \end{cases} \tag{2}$$

$$T(P) = \sum_{i=2}^{\infty} \sum_{j=-i}^{i} a^*_{ij} V^*_{ij}(P) \,, \tag{3}$$

cf. Heiskanen and Moritz (1967, Chp. 1 and 2).

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

$$L_i(T) = m_i, \qquad i = 1, \ldots, n \tag{4}$$

it is possible to find an approximation $\tilde{T}$ which agrees with observed quantities (i.e. eq. (4) is valid for $\tilde{T}$). This is provided the linear functionals L_i are elements of the space dual to a reproducing kernel Hilbert space of harmonic functions. $\tilde{T}$ will have the least norm, in between all elements of the space which fulfil eq. (4).

(We will in the following suppose that the reader is familiar with reproducing kernel Hilbert spaces. Otherwise we refer the reader to Davis (1975) or Meissl (1975, 1976)).

Let us denote the Hilbert space H. The inner product of two elements of H, f, g is denoted (f, g) and the norm of f, $\|f\|$, where $\|f\|^2 = (f, f)$. The dual space consist of all continuous, linear mapping from H to the real numbers, i.e. the linear functionals. This space will be denoted H'. The inner product of two elements of H', L_i and L_j is denoted (L_i, L_j) and the norm of L_i, $\|L_i\|$.

We will in the following suppose that the elements of H are functions harmonic in Ω and that H has a reproducing kernel, $K(P, Q)$. H will then be separable and there will exist a complete system of orthonormal elements spanning the space. Let us denote such a system by V_i, $i = 1, ..., \infty$. Then

$$K(P, Q) = \sum_{i=1}^{\infty} V_i(P)\, V_i(Q) . \tag{5}$$

For either P or Q fixed will the kernel be an element of H and linear functionals may therefore be applied on it. A linear functional L applied on the kernel with P or Q fixed will be denoted $L\,K(P,\cdot)$ and $L\,K(\cdot,Q)$, respectively. One further functional L' applied on one of these functions is denoted $L'L\,K(\cdot,\cdot)$.

The approximation $\widetilde{T}$ is then (cf. e.g. Tscherning (1975, section 2))

$$\widetilde{T}(P) = \sum_{i=1}^{n} a_i\, L_i\, K(P,\cdot) \tag{6}$$

with a_i, $i = 1, ..., n$ determined by the «normal» - equations

$$\{L_i\, L_j\, K(\cdot,\cdot)\} \quad \{a_i\} = \{m_j\}\, , i,j = 1, ..., n\, . \tag{7}$$

For the coefficients of the normal equation matrix we have cf. Davis (1975, Corollary 12.6.7))

$$L_i\, L_j\, K(\cdot,\cdot) = (L_i, L_j)\ , \tag{8}$$

and we see that the condition of $L_i \in H'$ is equal to the requirement that the diagonal elements of the matrix are finite. (We use

$$(L_i,L_i) = \|L_i\|^2 < \infty \Rightarrow L_i \in H')\ .$$

We also see, that it is required that the matrix is non-singular or equivalently that the linear functionals are linearly independent regarded as elements of H'.

When the number of observations increase, we can expect the linear functionals to be more and more dependent. This will be reflected in the numerical problems occuring when solving the equations (7). The problem is then how it can be assured that when increasing the number of observations we will (using the method of least squares collocation) obtain a sequence of approximations converging towards T.

This problem has been discussed in Moritz (1976, section 2), who proved that *strong* convergence can be assured for « regular » sets of observed boundary values of T, i.e. evaluated in a so-called ε-net covering the sphere. In the following sections we will give a general condition for convergence and give examples of Hilberts spaces where the use of regular sets of observations of values of T or of the gravity anomaly, Δg, situated at the boundary, will imply convergence.

2. — CONDITIONS FOR CONVERGENCE

Let us regard a set of observations

$$M = \{m_j, L_j(T) = m_j, L_j \in H', j = 1, ..., \infty\} \qquad (9)$$

with subsets

$$M_i = \{m_j \in M, j \leqslant i\}$$

for which the linear functionals L_j form a complete, linear independent set in H', i.e. they form a basis for H'.

The linear functionals may contingently be associated with specific points $\{P_i, i = 1, ..., \infty\ , P_i \in \Omega \cup \sigma\}$. This is for example the case when the functionals are a set of evaluation functionals, $L_i(T) = T(P_i)$. We will call the set of functionals a regular set when the associated point set forms an ε-net on σ. This means that there to each $\varepsilon > 0$ exist an integer N so that all point in σ has a distance less than ε to some point $P_j \in \sigma, j \leqslant N$.

There exists, as well known, a canonical isometric isomorphism $J : H' \to H$, which here is given by

$$J(L) = LK(\cdot, Q), \qquad L \in H', \qquad (10a)$$

so that

$$L(T) = (T(Q), LK(\cdot, Q)), \quad T \in H\ . \qquad (10b)$$

The functions $L_i K(\cdot,Q)$ will form a basis for H. We may from this basis construct an orthonormal base $\{V_i, i = 1, \ldots, \infty\}$ using the Gram-Schmit orthonormalization procedure. We will then have

$$V_i(P) = \sum_{k=1}^{i} c_{ik} L_k K(\cdot,P) . \tag{11}$$

When T is an element of H it may be represented by a series with respect to this basis

$$T(P) = \sum_{i=1}^{\infty} a_i V_i(P) , \tag{12}$$

$$\sum_{i=1}^{\infty} (a_i)^2 < \infty . \tag{13}$$

The coefficients of the series are

$$\begin{aligned} a_i &= (T(P), V_i(P)) \\ &= (T(P), \sum_{k=1}^{i} c_{ik} L_k K(\cdot,P)) \\ &= \sum_{k=1}^{i} c_{ik} L_k (T(P), K(P,Q)) \\ &= \sum_{k=1}^{i} c_{ik} L_k (T) = \sum_{k=1}^{i} c_{ik} \cdot m_k \end{aligned} \tag{14}$$

where we have used the reproducing property, the linearity of the inner product and eq. (10b).

Eq. (14) shows that the coefficients can be computed exclusively from the observed values. We can then suppose, that the set of observations consist of these coefficients a_i instead of the original values m_i. Let us then put

$$M' = \{a_i = (V_i(P), T(P)) = L_i' (T), \qquad i = 1, \ldots, \infty\} \tag{15}$$

$$M_i' = \{a_j, \quad j \leqslant i\} . \tag{16}$$

It is then obvious that

$$L_i' K(\cdot,P) = V_i(P) \tag{17}$$

and

$$L'_i L'_j K(\cdot,\cdot) = \delta_{ij} , \tag{18}$$

whereby using eq. (6) and (7) we see, that the approximation to T computed using M'_i is

$$\widetilde{T}_i(P) = \sum_{j=1}^{i} a_j V_j(P) . \tag{19}$$

Using eq. (13) we see that

$$\lim_{i \to \infty} \| \widetilde{T}_i - T \| = 0 , \tag{20}$$

i.e. $\widetilde{T}_i$ tend to T strongly. This also implies weak ($\approx$ pointwise) convergence because

$$| L_P(\widetilde{T}_i - T) | \leqslant \| \widetilde{T}_i - T \| \cdot \| L_P \| \to 0 , \tag{21}$$

where L_P is the evaluation functional associated with $P \in \Omega$, i.e. $L_P(T) = T(P)$.

When proving the strong convergence of $\widetilde{T}_i$ towards T it was essential that T was an element of H. In the current applications of least squares collocation T is not an element of H : When using the norm implied by the so-called empirical covariance function it has been proved in Tscherning (1977) that $T \notin H$. When the area of harmonicity is extended down to a so-called Bjerhammar-sphere inside the Earth, we only know that T may be approximated arbitrarily well by such functions in closed subsets of Ω, cf. Krarup (1969).

We could then hope to be able to prove weak convergence, e.g. by requiring T to be an element of another reproducing kernel Hilbert space H_0 which contains H as a subset.

It has not been possible to find a general proof of weak convergence in this case, but it is not so that weak convergence may not take place.

Suppose there exists an *orthonormal* base $\{V_i, i = 1, ..., \infty\}$ in H which forms an orthogonal base in H_0, i.e.

$$\left. \begin{aligned} (V_i, V_j)_0 &= 0 \qquad i \neq j \\ \| V_i \|_0^2 &= b_i^2 , \end{aligned} \right\} \tag{22}$$

where the subscript o indicates that we are regarding the inner product and the norm in H_o .

Let us then suppose that we are able to observe

$$a_i = (V_i, T), \qquad i = 1, \ldots, \infty . \tag{23}$$

Then

$$\tilde{T}_i(P) = \sum_{j=1}^{i} a_j V_j(P) , \tag{24}$$

but we do not know whether $\tilde{T}_i$ tends to T strongly. But as

$$\tilde{T}_i(P) = \sum_{j=1}^{i} (a_j b_j) b_j^{-1} V_j (P), \tag{25}$$

where $b_i^{-1} \cdot V_i(P)$ form an orthonormal base in H_o, and $\sum_{i=1}^{\infty} (a_i b_i)^2 < \infty$, (because $T \in H_o$), we see that $\tilde{T}_i$ tends to T strongly in H_o and thereby weak convergence is assured.

This indicates that it should be possible to have weak convergence when using collocation in a Hilbert space even if $T \notin H$ when the linear functionals associated with the observations form a complete set in both H' and H_o'.

3. — EXAMPLES OF HILBERT SPACES WHERE CONVERGENCE MAY TAKE PLACE

We will now try to characterize some Hilbert spaces in which collocation may determine a convergent series of approximations when boundary values of T or Δg are used. It is obvious that the first condition to be investigated is whether the linear functionals are elements of H'.

The spaces we will regard are all required to have reproducing kernels of the form

$$K (P, Q) = \sum_{i=o}^{\infty} \sigma_i \left(\frac{R^2}{r\, r'} \right)^{i+1} P_i (\cos \psi), \tag{26}$$

where r' is the distance of Q from the origin, ψ is the spherical distance between P and Q and P_i is the i'th Legendre polynomium. The σ_i are the so-called degree-variances which all are required to be positive.

The linear functionals related to the boundary values of T are the evaluation functionals at the boundary, L_P, i.e.

$$L_P (T) = T (P), \tag{27}$$

where P is a point on the boundary. The linear functionals associated with the gravity anomalies, $L_{\Delta g}$, are

$$L_{\Delta g}(T) = -\frac{\partial T}{\partial r}\bigg|_P - \frac{2}{R} T(P) . \tag{28}$$

Using eq. (26) and eq. (8) we have

$$\| L_P \|^2 = \sum_{i=o}^{\infty} \sigma_i \, . \, P_i (\cos o) = \sum_{i=o}^{\infty} \sigma_i \tag{29}$$

and

$$\| L_{\Delta g} \|^2 = \sum_{i=o}^{\infty} \frac{(i-1)^2}{R^2} \sigma_i . \tag{30}$$

Hence, in order to use boundary values of T or Δg must the degree-variances decrease towards zero at least like $i^{-1-\varepsilon}$ and $i^{-3-\varepsilon}$ for $\varepsilon > 0$, respectively.

In Tscherning (1972, 1973) are given explicit examples of Hilbert spaces with reproducing kernel. Here it is proved that

$$\| f \|_1^2 = \int_\sigma \sum_{i=o}^{3} \left(\frac{\partial f}{\partial x_i}\right)^2 d\sigma \tag{31}$$

imply $\sigma_i \approx i^{-1}$ and that

$$\| f \|_2^2 = \int_\sigma \sum_{i,j=1}^{3} \left(\frac{\partial^2 f}{\partial x_i \, \partial x_j}\right)^2 d\sigma \tag{32}$$

imply $\sigma_i \approx i^{-3}$. So we can see, that we must require at least $\|T\|_1 < \infty$ anp $\|T\|_2 < \infty$ in order to assure strong convergence using boundary values of T, Δg, respectively. That these and even stronger requirements are fulfilled seems likely considering the actually observed values of the first and second derivatives of T.

We finally need to prove that the linear functionals associated with the boundary values of T or Δg observed in a regular set of points may form a complete set. This will be the case when the corresponding boundary value problem has a unique solution for all elements of H and when the linear functionals are elements of H'. Hence for gravity anomaly observations the Hilbert space must not contain the three-dimensional subspace spanned by the first order solid spherical harmonics.

Let us first note, that when the evaluation functionals at the boundary are elements of H', then the boundary values of the elements of H will be continuous at the boundary. The same holds for the gravity anomalies at the boundary when the corresponding linear functionals are elements of H'.

Then suppose that there exists a linear functional $L \in H'$ which is ortogonal on the set of evaluation functionals at the boundary,

$$M' = \{ L_j \mid L_j(T) = T(P_j) \text{ for all } T \in H, j = 1, ..., \infty \}$$

where the points P_j form a regular set on σ. We must therefore according to eq. (10b) have

$$(LK(\cdot,Q), K(P_j, Q)) = LK(\cdot,P_j) = 0,$$

for all P_j. Now, the elements of H are continuous at the boundary and $LK(\cdot,Q)$ must therefore be zero at the boundary. Because of the required uniqueness of the boundary value problem it must be identically zero in Ω and the functional L must then be the zero-element of H'. This proves that the set M' is a complete subset of H'.

A similar proof can be given for the linear functionals associated with the gravity anomalies.

The above considerations can be summarized as follows :

We regard two Hilbert spaces $H_{1+\varepsilon}$ and $H_{2+\varepsilon}$ of functions harmonic in Ω and regular at infinity. From $H_{2+\varepsilon}$ we have removed the subspace spanned by the three first order solid spherical harmonics. We furthermore suppose that the reproducing kernels are given by eq. (26) with $\sigma_i \approx i^{-1-\varepsilon}$ and $\sigma_i \approx i^{-2-\varepsilon}$ for $H_{1+\varepsilon}$ and $H_{2+\varepsilon}$, respectively.

It is then obvious that in these spaces we have a unique solution of the boundary value problem with given values of T and Δg, respectively. Therefore, the two spaces are examples of Hilbert-spaces in which collocation may determine a convergent series of approximations to T, provided T is an element of the space.

4. — CONCLUSION

The discussion of strong or weak convergence of collocation may seem a little unfruitful. We will probably never be able to get a uniformly distributed, dense set of gravity anomalies and even if we got such a set the corresponding equations could probably not be solved.

However, investigations into the convergence conditions have made clear that even weak convergence is not assured using the empirical covariance function or Hilbert spaces of functions harmonic down to a Bjerhammar-sphere. And we have also been able to characterize some spaces where strong convergence may take place.

Still, may problems are open for future investigations.

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