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Construction of anisotropic covariance functions using Riesz-representers

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Abstract. A reproducing-kernel Hilbert space (RKHS) of functions harmonic in the set outside a sphere with radius R_0, having a reproducing kernel $K_0(P,Q)$ is considered (P, Q, and later P_n being points in the set of harmonicity). The degree variances of this kernel will be denoted σ_{0n}.

The set of Riesz representers associated with the evaluation functionals (or gravity functionals) related to distinct points $P_n, n = 1, \ldots, N$, on a two-dimensional surface surrounding the bounding sphere, will be linearly independent. These functions are used to define a new N-dimensional RKHS with kernel ($a_n > 0$)

$$K_N(P,Q) = \sum_{n=1}^{N} K_0(P_n,P) \cdot K_0(P_n,Q) \cdot a_n \tag{1}$$

If the points all are located on a concentric sphere with radius $R_1 > R_0$, and form an ϵ-net covering the sphere, and a_n are suitable area elements (depending on N), then this kernel will converge towards an isotropic kernel with degree variances

$$\sigma_n^2 = (2n+1)\sigma_{0n}^2 \cdot \left(\frac{R_0}{R_1}\right)^{2n+2} \cdot (\text{constant}) \tag{2}$$

Consequently, if $K_N(P,Q)$ is required to represent an isotropic covariance function of the Earth's gravity potential, $\mathrm{COV}(P,Q)$, σ_{0n} can be selected so that σ_n becomes equal to the empirical degree variances.

If the points are chosen at varying radial distances $R_n > R_0$, then an anisotropic kernel, or equivalent covariance function representation, can be constructed. If the points are located in a bounded region, the kernel may be used to modify the original kernel

$$\mathrm{COV}_N(P,Q) = \mathrm{COV}(P,Q) + K_N(P,Q) \tag{3}$$

Values of anisotropic covariance functions constructed based on these ideas are calculated, and some initial ideas are presented on how to select the points P_n.

Key words. Reproducing-kernel Hilbert Space · Gravity · Anisotropic · Non-homogeneous

1 Introduction

The anomalous gravity field of the Earth, T, may be described by a stochastic process, expressing its spatial variability (Moritz 1980; Sanso' 1986). The main tool has been the covariance (or coherence) function $C(P,Q)$, obtained by global integration of all values having a fixed spherical distance, ψ, equal to the distance between the points P, Q in space. Then

$$\mathrm{COV}(P,Q) = \sum_{i=2}^{\infty} \sigma_i^2 \left(\frac{R_2}{rr'}\right)^{i+1} P_i(\cos\psi) \tag{4}$$

where

$$\sigma_i^2 = \left(\frac{GM}{R}\right)^2 \cdot \left(\sum_{j=-i}^{i} C_{ij}^2\right) \tag{5}$$

are the degree variances; r, r' are the radial distances of P, Q respectively; ψ is the spherical distance between P and Q; P_i is the Legendre polynomial of degree i and C_{ij} are the normalized coefficients of T expanded in fully normalized solid spherical harmonics Y_{ij}. GM is the product of the gravitational constant and the mass of the Earth. All this is expressed in so-called spherical approximation, where the Earth is approximated by a sphere with radius R and $r = R + h$, h being the altitude of a point.

Corresponding to the stochastic process is an equivalent reproducing-kernel Hilbert space (RKHS) (Parzen 1959), where $\mathrm{COV}(P,Q)$ is the reproducing kernel, so that for an element f in the space

$$f(P) = \langle f(Q),\ \mathrm{COV}(P,Q)\rangle \tag{6}$$

$\langle \cdot, \cdot \rangle$ being the inner product. Just as the covariance function due to its construction is isotropic, the inner product will have the same property. (For a definition of isotropy and homogeneity on the sphere, see Grafarend et al. 1985.) The covariance of two linear functionals of the same kind, L_P, L_Q

$$K(L_P, L_Q) = \mathrm{COV}(L_P, L_Q) = \langle L_P, L_Q \rangle^* \tag{7}$$

will then be constant for pairs of points, which can be mapped into each other by a rotation of $\mathbf{R}^3$ around its origin [the * on the inner product in Eq. (7) indicates that it is the inner product in the dual space].

This is to a certain extent unsatisfactory, because it gives a statistical description of T as being homogeneous, while in reality both the variance and the correlation length changes with location (see e.g. Grafarend 1971a, b; Lachapelle and Schwarz 1980; Schwarz and Lachapelle 1980; Goad et al. 1984). As a consequence, the use of isotropic kernels or covariance functions in an optimal least-squares estimation procedure like Kriging or least-squares collocation (LSC) does not give optimal results (see, for example, Kearsley 1977; Tornatore and Migliaccio, submitted).

It also makes the signal-to-noise ratio a constant for fixed noise and fixed altitudes and functionals. It is even the case that in mountains the variance decreases with altitude, which is not likely. This is a draw back when an isotropic covariance function is used in Kriging or LSC.

There is a possible solution to this problem, which will be described below.

2 The problem of anisotropy and non-homogeneity

There are several solutions to the problem of anisotropy and non-homogeneity (in the following, anisotropy will be used to cover both concepts).

2.1 The Danish method

This method aims at making the gravity field look like it does in Denmark everywhere, i.e. very smooth and homogeneous. This is achieved through the so-called remove–restore method (Forsberg and Tscherning, 1981), where everything known is subtracted (like the attraction of mountains or density anomalies) and later added back. This gives a homogeneous field (see Schwarz and Lachapelle 1980; Forsberg 1986; Arabelos and Tziavos 1995).

2.2 The anisotropic covariance model method

Here, the aim is to find a more general expression for the covariance function, which will, for example, show a directional dependence (see, for example, Rummel and Schwarz 1977). One method used in Kriging also uses a set of covariance functions (or variograms), depending only on the distance, but being different for, e.g., each 15 degrees of azimuth.

Clearly, the two methods outlined above are not mutually exclusive. Below, a method will be proposed which may be used to describe quite a general statistical behaviour. It should also make LSC more competitive with other methods which (sometimes implicitly) build on anisotropy, by using non-homogeneous sets of base functions in a least-squares procedure, such as potentials of mass points, where the mass points are buried at varying depths (see, for example, Barthelmes and Kautzleben 1982; Bathelmes 1986). In addition, the use of Fourier series is not hampered by anisotropies, except sometimes in the gridding step, which often uses LSC for the generation of the grid values.

3 General covariance models

The method used to handle anisotropies has been to use different isotropic covariance functions in different (mostly fixed) areas. This creates a problem at the area boundaries, because the spectral relationships (between different types of functionals) are 'fractured' (see, for example, Tscherning et al. 1987). We need a covariance function which smoothly changes its spectral relations.

The method used to analytically represent different covariance functions may hint at how this could be achieved. One frequently used method for representing the spectral behaviour for the degree tending to infinity is to use linear combinations of exponential- and polynomial-type expressions for the degree variances (Lauritzen 1973; Tscherning and Rapp 1974; Jekeli 1978)

$$\sigma_{0n}^2 = \sum_{i=1}^{k} \left(\frac{R_i^2}{R^2} \right)^{n+1} \frac{\mathrm{Pol}_{1i}(n)}{\mathrm{Pol}_{2i}(n)} \tag{8}$$

In the so-called T/R models, $k = 1$, Pol_{1i} is a constant and Pol_{2i} is a polynomial of degree 2, 3 or 4 in n, and R_1 is the radius of the Bjerhammar sphere. We will in the following only consider models of this type.

Generally, the variance $\mathrm{COV}(L, L)$ will increase if R_1 is close to R, and the half-correlation distance will decrease. Intuitively, this corresponds to becoming closer to or further away from the disturbing masses.

One could, therefore, initially prescribe Bjerhammar surfaces which changed as a function of location (see Fig. 1). This, however, would lead to non-harmonic covariance functions, but could obviously be used to describe statistical properties for other phenomena than potential fields.

For T we could try to construct an RKHS by orthonormalizing the solid spherical harmonics with respect to such a surface using a standard Sobolev inner product. Since the solid spherical harmonics will not be orthogonal in such a space, the orthonormal basis will consist of linear combinations of functions with a lower index, supposing standard Gram–Schmidt orthonormalization is used. The reproducing kernel (= the covariance function) would then be

$$\mathrm{COV}(P, Q) = \sum_{i=1}^{\infty} \sum_{j=-i}^{i} \sum_{k=1}^{\infty} \sum_{l=-k}^{k} \sigma_{ijkl} Y_{ij}(P) \cdot Y_{kl}(Q) \tag{9}$$

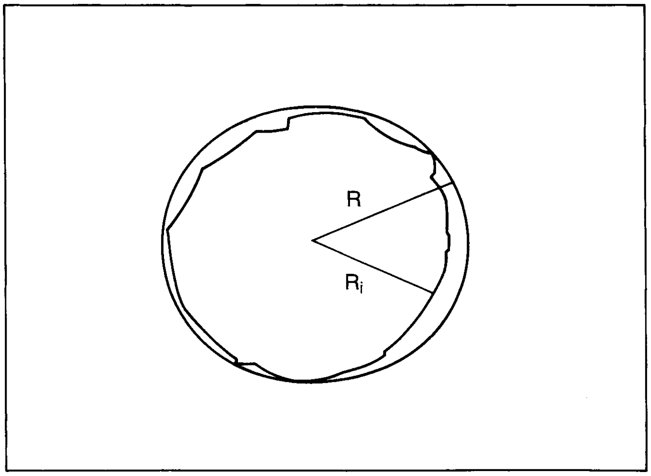

Fig. 1. Bjerhammar surface inside mean-Earth sphere

Note that here one would certainly lose the possibility of evaluating the covariances using closed expressions like we have for the models given above [Eq. (8)].

Now write

$$\mathrm{COV}(P,Q) = \sum_{i=1}^{\infty}\sum_{j=-i}^{i}\sigma_{ij}Y_{ij}(P)\cdot\sum_{k=1}^{\infty}\sum_{l=-k}^{k}\sigma_{kl}Y_{kl}(Q) \tag{10}$$

and suppose we could find a point P_S so that

$$\sigma_{ij} = \sigma_{kl} = Y_{ij}(P_S)\cdot f(i) \tag{11}$$

Then

$$\mathrm{COV}(P,Q) = \sum_{i=1}^{\infty} f(i)(2i+1)P_i(\cos\psi_{PP_i}) \cdot\sum_{k=1}^{\infty} f(k)(2k+1)P_k(\cos\psi_{P_kQ}) \tag{12}$$

and if $f(i)$ could be parameterized using Eq. (7) then $\mathrm{COV}(P,Q)$ could be evaluated as a product of closed expressions.

Now, it is quite unlikely that this would be possible. But what about sums of expressions for sets of points P_S covering the whole Earth, and being associated with various depths? For such a finite set the functions are linearly independent because they may be regarded as a set of so-called Riesz representers of the evaluation functionals associated with the points. (A Riesz representer is a function which has the property that the inner product of the representer and an arbitrary function in the RKHS gives the value of the quantity represented by it. Examples are the value in a point or the value of the gravity anomaly in the point. See, for example, Tscherning 1985, p. 284.)

One may define the inner product by declaring the functions orthonormal. The reproducing kernel would be harmonic and expressible as given in Eq. (1). (The evaluation functionals could be substituted by an equivalent set of functionals, such as gravity anomaly functionals.)

Since this is correct it should be possible also in the isotropic case, and we will prove this now in the limit. Suppose we have sets of N (equidistant) local points P_n all associated with the same Bjerhammar sphere with radius R_1. When N increases the points become closer and closer.

If we select

$$f_i = \sigma_{0i}\cdot\frac{1}{\sqrt{2i+1}} \tag{13}$$

then in the limit the sum will become the integral (over the unit sphere) supposing the weights are selected equal to the area elements:

$$\begin{aligned}\lim_{N\to\infty}&\sum_{n=1}^{N}\sum_{ij}^{\infty} f(i)Y_{ij}(P)Y_{ij}(P_n)\\ &\cdot\sum_{kl}^{\infty} f(k)Y_{kl}(Q)Y_{kl}(P_n)a_n\\ &=\sum_{ij}^{\infty}\sum_{kl}^{\infty} f(i)f(k)\cdot\int Y_{ij}(P_n)Y_{kl}(P_n)\,\mathrm{d}s\cdot Y_{ij}(P)Y_{kl}(Q)\\ &=\sum_{ij}^{\infty} f(i)^2 Y_{ij}(P)Y_{ij}(Q)\\ &=\sum_{i=1}^{\infty}\sigma_{0i}^2\left(\frac{R^2}{rr'}\right)^{i+1}P_i(\cos\psi_{PQ})\end{aligned} \tag{14}$$

Consequently, we are able to approximate an 'old' isotropic covariance function by a finite sum of kernels of a similar family. The space will be of finite dimension, so we need at least as many points as the number of observations if the kernel is to be used in LSC. Alternatively, we could use the sum of an old kernel and the finite one, cf. Eq. (3).

Note the similarity between LSC and point-mass methods, if the data points and the point masses are suitably selected.

4 Preserving the spectral relationship

In LSC it is possible to use a mixture of different data types, such as geoid and gravity values, when estimating T. In local applications it is important to have consistency between the variances of the functionals, i.e. to have a correct model for the degree variances for both a low degree as well as when the degree tends to infinity. One can see from Eq. (10) what one must do, and numerical tests have shown that the spectral relationship may be preserved, at least to a certain degree.

The covariance function used for tutorial purposes for the New Mexico White Sands area (Tscherning 1994) has been used as an example. Time has not permitted the writing of new software, so old programs and models have been used. For the degree variances above degree 360 we use

$$f(i) = \frac{A}{\sqrt{2}(i-1)(i-2)}\left(\frac{R_1}{R}\right)^{i+1} \tag{15}$$

so that

$$\sigma_i^2 \approx \frac{A^2}{i^3}\left(\frac{R_1}{R}\right)^{2i+2} \tag{16}$$

For degrees below 361, the square root of the error degree variances multiplied by the square root of $2n+1$ was used. A scale factor was also used so that the gravity anomaly variance became correct.

In Table 1 are shown the old values at an altitude of 1700 m, and the new values calculated from only one functional, i.e. $N = 1$. The reason that the location of the first zero is much larger for the low derivatives is obviously that, by taking the square root of the quantities, the low degrees are given larger weight. There are, however, many tools to adjust the model so that reasonable spectral relationships can be preserved.

5 Selection of the points P_n

Exercise: show that the RKHS with kernel $K_1(P,Q) = K_0(P,P_1)K_0(Q,P_1)$ is one-dimensional.

If we use a modified kernel as given in Eq. (3), then it is enough to select just one point, since the space will be infinite-dimensional. If not, then we must select at least as many points as observations, if the kernel is to be used in LSC. These points could be distributed in a regular grid covering the area where LSC is used. The grid density should be so large that the variance for points inside the grid does not decrease very much, probably not more than 10%. The depths of the points could be selected using variances calculated by sampling data in a fixed area around the point. However, we often find that the variance does not change very much between geological provinces. Consequently, all depths could be equal in a statistically homogeneous area.

No numerical tests have yet been carried out, so the solution of the problem is still open.

6 Conclusion

In general, the 'Danish method' (cf. Sect. 2) will give satisfactory results. However, in such cases as when the density variations are due to sources located below the surface, or where a reliable digital terrain model is not available or of insufficient quality, the use of non-isotropic kernels may improve the results when using LSC or similar norm-minimization methods.

Here, the mathematical basis for constructing anisotropic kernels and covariance functions has been provided. The use of this tool is now being studied, in particular algorithms for selecting the location of the points associated with the functionals.

The estimation of anisotropic covariances also needs to be studied further. How large should the sampling areas be for the estimation of the variance and the correlation length?

It is hoped that Lauritzen's prediction (Lauritzen 1973) that it becomes more difficult to estimate the covariance function than to find a suitable approximation to the anomalous gravity potential is proved to be incorrect.

Table 1. Variances and correlation distances for old and new covariances

	Geoid		Gravity		T_{zz}	
	Old	New	Old	New	Old	New
Variance	0.0652	0.142	142.2	142.2	150.04	236.65
Half-correlation	0.39	2.1	0.16	0.95	0.09	0.065
Zero correlation	4.15	22.4	0.32	0.34	0.21	0.25

The points P, Q have heights equal to 1.7 km, and the point P_1 is at a depth of 1.7 km. Units: geoid variance, m^2; gravity, mgal^2; second-order vertical derivative T_{zz}, EU^2. The correlation distances are given in decimal degrees

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