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Isotropic Reproducing Kernels for the Inner of a Sphere or Spherical Shell and Their Use as Density Covariance Functions[1]

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Isotropic reproducing kernels for a sphere or spherical shell are derived as weighted product sums of L_2 orthonormal base functions. For the sphere these functions are product5 of the surface spherical harmonics and the Jacobi polynomials of degree (0, 2). Reproducing kernels for a sphere are consistent with the covariance function of the outer anomalous gravity potential of the Earth. These reproducing kernels may be used for gravity field modeling which include density (anomaly) data as observations or which aims at predicting such quantities using optimal estimation methods, that is for solving the inverse gravimetric problem.

KEY WORDS: gravity. Earth's density distribution, covariance functions, reproducing kernel

INTRODUCTION

A separable Hilbert space of functions $f : w \subseteq \mathbb{R}^3 \rightarrow \mathbb{R}$ will have a reproducing kernel, $K(P, Q)$, if the evaluation functionals are continuous. P and Q are points in ω. If the space has an inner product (,) and f is an element of the space, then $(f(P), K(P, Q)) = f(Q)$.

The reproducing kernels also may be interpreted as covariance functions of stochastic processes (see, for example, Parzen, 1975). The covariance functions are needed in optimal estimation, and may be used to solve inverse problems if the cross-covariance function between the "signal" and the "source" can be determined. Unfortunately, this generally requires that the inverse problem has been solved. But a step on the way is to establish possible covariance functions. Conversely, empirically estimated covariance data may be used to select a reproducing kernel, which when used in the method of collocation (or kriging) for the approximation of a function, gives a result which in a statistical sense is optimal. This is the motivation for the following derivations.

We will derive expressions for a large class of covariance functions of

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integrable functions having support inside a sphere or a spherical shell. In earlier work (Tscherning, 1977), expressions for covariance functions of a so-called quasiharmonic type have been derived. Quasiharmonic functions are functions which after multiplication with a function only depending on the radial distance r, fulfil1 the Laplace-equation. Each class of these functions have a one-to-one relationship to the set of functions harmonic outside a sphere (Tscherning and Suenkel, 1981).

Unfortunately the use of these functions constrained the inverse solutions too much (see Hein and others, 1989). For example, the mass density distribution would be concentrated close to the surface of the sphere. One of the reasons for this was that the correlation as a function of depth difference for spherical distance zero always was positive. And again the reason for this was that the base functions used had not been orthonormalized over the interval from zero to R, where R is the radius of the sphere, nor over the interval from a to b bounding a spherical shell.

ISOTROPIC REPRODUCING KERNELS

In the following, we will discuss only isotropic reproducing kernels, that is kernels which depend on the spherical distance ψ and on the distances r, r' of P. respectively Q from the origin. (The latitude and the longitude of P, Q will be denoted by p, X and p', X', respectively.)

If an isotropic inner product is used, then an isotropic kernel is obtained. Therefore, we may start with the usual L, norm. This kernel, however, does not in itself lead to a reproducing kernel because its value for P identical to Q will be infinite. (The value of the kernel for P equal to Q is equal to the square of the norm of the so-called evaluation functionals, which is required to be finite.) But a kernel may be constructed as the product sum of the functions in the orthonormal base f_{ijk} evaluated in P and Q and multiplied by positive constants (variances) σ_{ijk} such that the sum becomes finite when evaluated in (P, P).

The base functions may be determined using Gram–Schmidt orthonormalization of all polynomials $x^i y^j z^k$, or equivalently $r^k Y_{ij}(\varphi, X)$, where the Y-functions are the usual surface spherical harmonics, normalized over the unit sphere, $-i \le j \le$ i, [cf. Heiskanen and Moritz, 1967, Eqs. (1–73)]. Here instead of r we will use a new variable $x = (r-a)/(b-a)$, which for the sphere becomes x $= r/R$. (For an extended discussion of base functions, see Ballani. Engel, and Grafarend. 1993.)

The Y-functions are orthonormal (except for a factor 4π) over the unit sphere. We therefore need only to orthonormalize the polynomials x^k over the interval from a to b with the weight function $(x + a/(b-a))^2$. If we introduce a new variable $y = (x + 1)/2$ to switch to the interval from -1 to 1 we see that the weight function becomes $(y + 1)^2/2^3$ for the sphere ($a = 0$ and $b = R$). Hence the orthononnal functions are the Jacobi polynomials of the type (0, 2) (see, for example, Davis. *1975*, p. *366*). For an interval we also obtain orthogonal polynomials, but with slightly more complicated expressions than what we get for the sphere. We will discuss here only the sphere, but all properties discussed hold for a spherical shell as well.

As functions of x the Jacobi polynomials are simple polynomials in x and $x - 1$ of maximal degree k in x. We select the functions $J_k(x)$ so that they are the Jacobi polynomials of type $(0, 2)$ and polynomial degree k in x, but equal to 1 for $x = 1$. Then

$$J_0(x) = 1, J_1(x) = 4x - 3, \text{ and } J_2(x) = 15x^2 - 20x + 6$$

A polynomial of degree k will have k zero-points in the interval from 0 to 1. The equivalent normalized functions are obtained by multiplication with a factor $(2k + 3)^{1/2}$. They fulfill a simple recursion fonnula (Davis, *1975,* p. 366),

$$J_{k+1}(x) = (a_k x + b_k)J_k(x) + c_k J_{k-1}(x)$$

with

$$a, = (2k + 1)2(k + 2)(k + 1)/d_k,\ b_k = -(k^2 + 3k + 3)/d_k$$

$$b_k = -k(k + 2)^2/d_k, \text{ and where } d_k = (k + 1)^2(k + 3)$$

Similar 3-term recursion formulae exists if we had orthonormalized over the interval from a to b.

KERNELS FOR THE SPHERE

The general isotropic reproducing kernel for a sphere then becomes

$$K(P, Q) = \sum_{i=0}^{m} \sum_{j=-i}^{i} \sum_{k=0}^{m} \sigma_{ik}(2k + 3)Y_{ij}(\varphi, \lambda)Y_{ij}(\varphi', \lambda')J_k\left(\frac{r}{R}\right) J_k\left(\frac{r'}{R}\right)$$

After summation over j we get (using the well-known relationship between product-sums of surface spherical harmonics of the same degree i and the Legendre polynomials P_i with argument equal to cosine of the spherical distance [cf. Heiskanen and Moritz, *1967,* Eq. (1–82)]).

$$K(P, Q) = \sum_{i=0}^{\infty} (2i + 1)P_i(\cos \psi) \sum_{k=0}^{i} \sigma_{ik}(2k + 3)J_k\left(\frac{r}{R}\right) J_k\left(\frac{r'}{R}\right)$$

(Note that the summation with respect to k terminates at $k = i$. This will be justified in the following.) If we select the constants σ_{ik} so that they are independent of k, then we may use our knowledge about the external gravity field to determine the constants.

Using Newtons inverse square law twice we obtain the relationship between the covariance function (reproducing kernel) of the outer potential T and the "inner" kernel K.

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

$$= G^2 \int\int \frac{K(S,S')}{\|P-S\| \,.\, \|Q-S'\|} dS\, dS'$$

where S and S' are points inside the sphere and $\|P - S\|$ and $\|Q - S'\|$ are the distances between the points. G is the Newtonian gravity constant.

After some simple derivations where we use that the reciprocal distance may be expanded as a series in Legendre polynomials [see Heiskanen and Moritz, 1967, Eq. (1–80)] we get

$$\mathrm{cov}(T(P),\ T(Q)) = (G \cdot 4\pi \cdot R^2)^2 \sum_{i=0}^{\infty} P_i(\cos\psi)$$

$$\cdot \sum_{j=0}^{i} \frac{2j+3}{2i+1} (I_j^i)^2 \left(\frac{R^2}{rr'}\right)^{i+1} \sigma_{ij}$$

with

$$I_j^i = \int_0^1 \left(\frac{r}{R}\right)^i J_j\left(\frac{r}{R}\right)\left(\frac{r}{R}\right)^2 d\left(\frac{r}{R}\right)$$

This integral is easy to calculate using the recursion formula for $J_k(x)$, which is valid for I_j^i. For i $< j$ we will obtain $I_j^i = 0$ because of the fact that the functions J_i are obtained by orthonomalization of x^i. This explains the use of a finite upper summation limit for the J_i functions.

Several global covariance models have been proposed for the external gravity potential (Tscherning and Rapp, 1974; Tscherning, 1976: Moritz, 1977; Jekeli, 1978). Using the models number 2 and 3 of (Tscherning, 1975) we have

$$\sigma_i^T = \frac{s^{i+1} \cdot A}{(i-1)(i-2)f(i)} = \sum_{j=0}^{i} \frac{2j+3}{2i+1} (I_j^i)^2 (G \cdot 4\pi \cdot R^2)^2 \sigma_{ij}$$

with $f(i) = (i + B)$ (Model 2) and $f(i) = (i + B)(i + C)$ (Model 3), we may determine σ_{ij} under the condition that σ_{ij} is independent of j. Here, we will use $\sigma_j = \sigma_{ij}(2j + 3)$. The values of σ_i are shown in Figure 1 for Model 3, where B = 13, C = 1100, $A = 465110.0{*}R^2$, and $s = 0.995$.

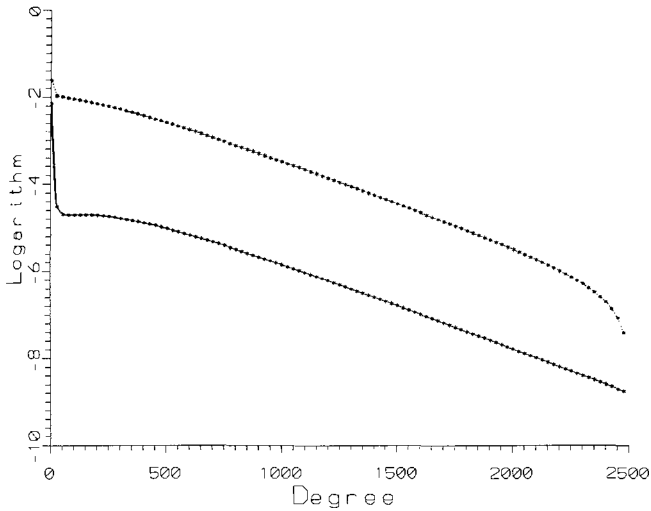

Figure 1. Lowermost curve shows logarithm of variances and uppermost curve shows logarithm of accumulated variances from degree *2500* to degree *2* for Model *3*.

By putting $\sigma_{ik} = 0$, i $\leq$ N and starting the summation over *j* at a value M > 0, we may obtain models with differing correlation distances and position of the first zero crossing. This has become possible because of the location of the zeroes of the Jacobi polynomials.

Figure 2 illustrates this for Model 2 and 3. We have evaluated $K(P, Q)$ for $\psi = 0$, $r' = R$ and r varying from R to 0. For model 3 we have used the same constants as used to calculate the values in Figure 1. For Model 2 we have used B = 24, $A = 425.28*R^2$, and again $s = 0.995$. The summation started for N = M = 5 and terminated at i = 4500. The corresponding gravity anomaly variances are 801 $mgal^2$ for Model 2 and 947 mgal' for Model 3. (These values are reasonable for an Earth without isostatically compensated topography.)

KERNELS FOR SPHERICAL SHELLS

Kemels for spherical shells will have the same form as we have seen, but the more general Jacobian functions must be used. If we want to model the Earth using a sphere filled with a number, n, of spherical shells (see, e.g., Arnold and Schoeps, 1984). then this is possible. In this manner we can model a layered Earth. However, the densities in the layers may be correlated. This can be modeled prescribing the correlation between points in the layers using a $n \times n$ covariance matrix, (see, e.g., Knudsen, 1993). It becomes then rather

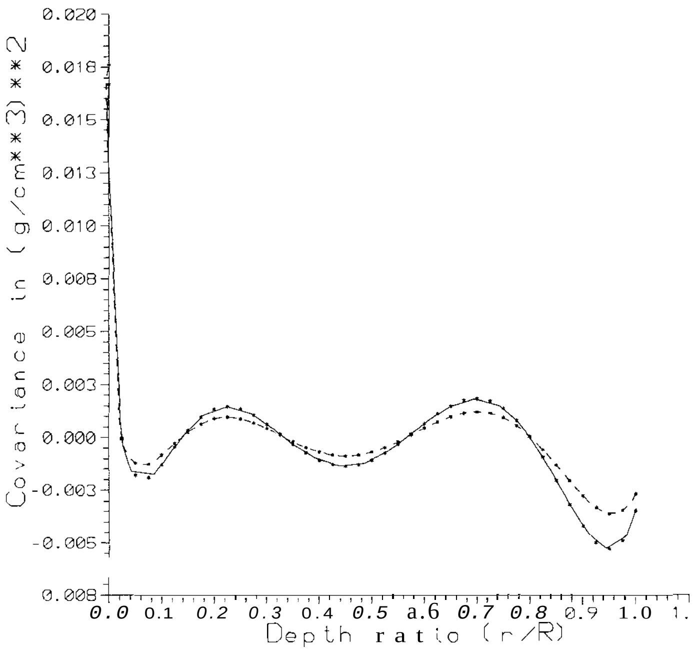

Figure 2. Density covariance function for $r' = R$ and depth-ratio $d = (R - r)/r$ between 0 and 1. Covariances shown for Model 3 by solid curve and for Model 2 by dashed curve. Lower summation limit used was equal to 5 and upper limit equal to 4500.

difficult to use the statisical information about the outer potential, without also having a priori estimates about the correlation between the layers.

CONCLUSION

We have shown that here we have a flexible tool for the analytic representation of density covariance functions for a sphere consistent with the covariance functions of the outer gravity potential. However, be aware that the values used to generate the two figures are one of the choices which seem to give reasonable values of the density (anomaly) variation at the Earth's surface. Other selections could have given completely absurd values.

Further analysis is necessary in order to select a reasonable weight-ratio between the Jacobi-polynomials and the Legendre functions, that is the depth correlation scale as compared to the horizontal distance correlation. Thus, in practice, it is necessary to select a proper functional dependence for the variances σ_{ij} as a function of j.

If the density distribution is modeled using spherical shells, a hypothesis about the correlation between shells must be formulated, similar to those known from isostatic theory. Or, we may be able to estimate the correlations for shallow depths from well-log data.

It is scary to see that simple functions, which seem similar to probable density distributions, have zero outer gravity potential. Which additional information will be needed to determine these components of the density distribution?

Exercise. Show that the density function $d(r) = 4*(r/R) - 3$, $r < R$ has zero outer potential.

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