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Isotropic reproducing kernels for the inner of a sphere and their use as density covariance functions

by

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A separable Hilbert space of functions $f:\omega \subseteq \mathbb{R}^3 \rightarrow \mathbb{R}$ 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 may also be interpreted as covariance functions of stochastic processes, see e.g. 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 found. Unfortunately this generally requires that the inverse problem has already been solved. But a step on the way is to establish **possible** covariance functions. This is the motivation for the following derivations, where we will derive expressions for a large class of covariance functions of integrable functions having support inside a sphere or a spherical shell. In earlier work (Tscherning, 1977) expressions for covariance functions of so-called quasi-harmonic type have been derived. Unfortunately these functions constrained the inverse solutions too much, see Hein et al.(1989). One of the reasons for this were that the correlation as a function of depth difference for spherical distance zero always was positive. And again the reason for this were that the base functions used had not been orthonormalized over the interval from zero to R, where R is the radius of the sphere, neither on the interval R_i to R_{i+1} bounding a spherical shell.

We will in the following only discuss isotropic reproducing kernels, i.e. they only 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 φ, λ and φ', λ', respectively).

If an isotropic inner product is used, then an isotropic kernel is obtained. We may therefore start with the usual L_2 norm. The kernel will then be the product sum of the functions in the orthonormal base f_{ijk} evaluated in P and Q. New isotropic kernels are then obtained by multiplying each term with positive constants (variances) σ_{ijk}.

The base functions may be found using Gram-Schmidt orthonormalisation of all polynomials $x^i y^j z^k$, or equivalently $r^k\ Y_{ij}(\varphi,\lambda)$, where the Y-functions are the usual surface spherical harmonics, normalized over the unit sphere, $-i \leq j \leq i$. In the following we will instead of r use a new variable x = r/R. A similar variable could have been introduced for the spherical shell. However we limit the following derivations to the full sphere, and the shell is left as an exercise to the reader. (Note that models for plane layers have been developed e.g. by Knudsen (1993)).

The Y-functions are already orthonormal (except for a factor 4π) over the unit sphere. We therefore only need to orthonormalize the polynomials x^k over the interval from zero to one with the weight function x^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 $(y+1)^2/2^3$. Hence the orthonormal functions are the Jacobi polynomials of degree (0,2), see e.g. Davis (1967). As functions of x they are simple polynomials in x and x-1 of maximal degree k. If we select the functions $J_k(x)$ so that they are equal to 1 for x = 1 then

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

A polynomial of degree k will have k zero-points on the interval from 0 to 1. The equivalent normalized functions are obtained by multiplication with a factor $(2k+3)^{1/2}$. They fulfil a simple recursion formula,

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

$a_k = (2k+1)2(k+2)(k+1)/d_k$, $b_k = -(n^2 + 3n + 3)/d_k$,
$b_k = -k\,(k+2)^2/d_k$, and where $d_k = (k+1)^2(k+3)$.

Similar 3 - term recursion formulae exists if we had orthonormalized over the interval from R_i to R_{i+1}.

The general isotropic reproducing kernel then becomes

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

After summation over j we get

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

(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} equal to a known function of k, then we may use our knowledge about the external gravity field to determine the constants. The covariance function (reproducing kernel) of the outer potential T is

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

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

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 reciproc distance may be expanded as a series in Legendre polynomials) we get

$$cov(T(P),T(Q))=(G \cdot 4\pi \cdot R^2)^2 \sum_{i=0}^{\infty} P_i(\cos\psi) \cdot \sum_{j=0}^{i} \frac{2j+3}{2i+1} \left(I_j^i\right)^2 \left(\frac{R^2}{rr'}\right)^{i+1} \sigma_{ij}$$

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 also valid for I^i_j. For $i < j$ we will obtain $I^i_j = 0$ due to the fact that the functions J_i are obtained by orthonomalisation of x^i. This justifies the use of a finite upper summation limit for the J_i functions.

Using one of the models (Tscherning, 1975) we have

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

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 $\sigma_i = \sigma_{ij}(2j+3)$. 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.

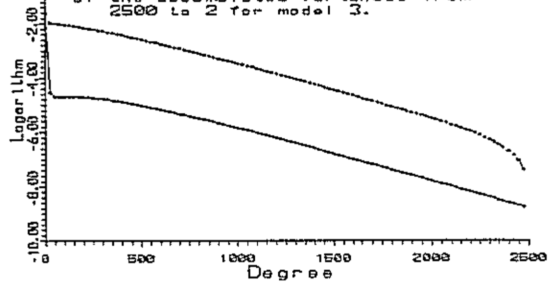

Figure 1. Lowermost curve shows the logarithm of the variances and the uppermost curve shows the logarithm of the accomulated variances from 2500 to 2 for model 3.

By putting $\sigma_{ik} = 0$, $i \leq N$ and starting the summation over j at a value M > 0, we may obtain models with varying 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^2 for model 3. (These values are reasonable for an Earth without isostatically compensated topography).

In conclusion, this shows that we here have a flexible tool for the analytic representation

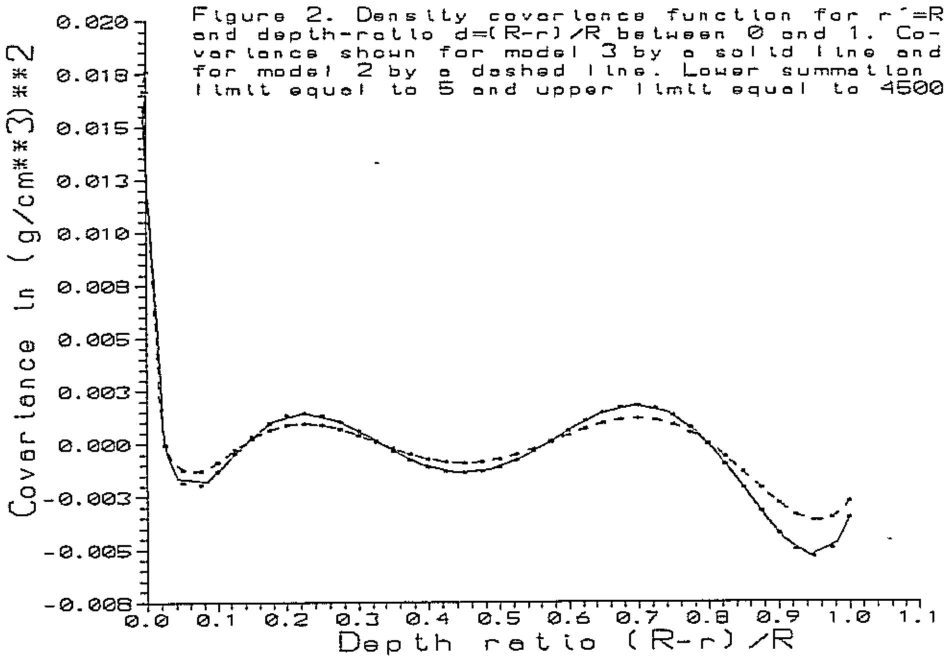

Figure 2. Density covariance function for r´=R and depth-ratio d=(R-r)/R between 0 and 1. Covariance shown for model 3 by a solid line and for model 2 by a dashed line. Lower summation limit equal to 5 and upper limit equal to 4500.

of density covariance functions 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 choices 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, i.e. the depth correlation scale as compared to the horizontal distance correlation. This means in practice to select a proper functional depencence for the variances σ_{ij} as a function of j.

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

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