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Density–gravity covariance functions produced by overlapping rectangular blocks of constant density

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SUMMARY

A set of N rectangular blocks of unit density form the basis of a linear vector space. This space will be a Hilbert space with reproducing kernel, when equipped with the L_2 norm (and inner product). The kernel, $K(P, Q)$, will be the product sum of the (maximally N) orthonormalized base functions evaluated at two points P, Q, in space. Multiplied by an appropriate scaling constant, this function will be a covariance function for a random density (anomaly) function. Using covariance propagation, auto- and cross-covariance functions for and with quantities related to the (anomalous) gravity field created by the random density function may be computed.

When blocks of varying volume are used, the density variance will vary within the structure described by the blocks. For disjoint blocks, the variance is inversely proportional to the volume. The use of overlapping blocks generally creates correlations between density values in different blocks, a possibility which does not exist when using disjoint blocks.

Computational examples are presented which show that it is possible to create realistic covariance models for the gravity anomaly, and that the cross-correlation between surface gravity and surface density may obtain values in the interval from 0.4 to 0.7. These values are more realistic than values obtained in earlier studies using quasi-harmonic density models.

Key words: covariance, density, gravity.

1 INTRODUCTION

Let us suppose that we have available a reference (mass) density distribution, ρ_0, consistent with an external reference potential, U. The anomalous potential, T, is then equal to $W - U$, where W is the gravitational potential of the Earth. We will suppose that it is equal to the potential produced by the anomalous density distribution (density contrast), ρ.

The general inverse gravimetric problem is the problem of the determination of an estimate of ρ from values of linear functionals applied on T or on ρ. Examples of values of such functionals are the density at a point, $\rho(P)$, and the gravity anomaly Δg at a point Q.

Various methods exist for the solution of this problem (Sansò & Tscherning 1989). Most methods require the estimate of ρ to be an element of a (finite- or infinite-dimensional) linear vector space. Two extreme cases are (1) a space having as elements fixed blocks of equal density and (2) a space consisting of harmonic functions inside a sphere (Tscherning 1974). Frequently, iterative methods are used where a new vector space is used in each step, e.g. with changed locations of the blocks of equal density. Here the unknowns may be the values of parameters describing the location of block boundaries. We will not discuss such iterative methods here, but only the 'linear' case, which is often the problem to be solved in each iteration step.

The linear methods may be classified according to whether the dimension (N) of the vector space is larger, equal to, or smaller than the number of observations (m) used. An analysis of the three cases (see Sansò, Barzaghi & Tscherning 1986; Tscherning 1986; Tscherning, Forsberg & Vermeer 1990) shows that they may all be given a statistical interpretation. The density may be viewed as a second-order random function with a certain autocovariance function. Correspondingly, the method of solving the inverse gravimetric problem may be interpreted as a method of optimal linear estimation. A somewhat surprising result is that 'clean' deterministic methods may also be given a statistical interpretation.

The direct use of optimal estimation as discussed in e.g.

Jackson (1979) gives difficulties. One generally needs to specify the autocovariance of the density values at two points P, Q, $\mathrm{cov}[\rho(P), \rho(Q)]$, and the cross-covariance function of the density and the observed quantity, such as the gravity anomaly, Δg, or the gravity disturbance, δg.

The covariance function, $\mathrm{cov}[\rho(P), \delta g(Q)]$ is obtained from $\mathrm{cov}[\rho(P), \rho(Q)]$ using the functional relationship between δg and ρ, i.e.

$$\mathrm{cov}[\rho(P), \delta g(Q)] = -G \int \frac{\partial}{\partial r} \{\mathrm{cov}[\rho(P), \rho(R)]/\|R-Q\|\}\, dR, \quad (1)$$

where G is the gravitational constant, R is a point inside the masses, $\|R-Q\|$ is the distance between the points Q, R and the partial derivative with respect to the radial distance, r, is evaluated at the point Q. The autocovariance function of two gravity disturbances is obtained by integrating and differentiating once more as in equation (1).

To the knowledge of the author, there are very few classes of functions which have elements which simultaneously may be used as models for the covariance, $\mathrm{cov}[\rho(P), \rho(Q)]$, and for which the expression (1) may be evaluated analytically. One of the few classes of functions are those which after a multiplication by two functions of the radial distance to P, Q, respectively, become harmonic functions (Tscherning 1977; Tscherning & Sünkel 1981).

The use of these so-called quasi-harmonic functions for the solution of the inverse gravimetric problem was investigated in Hein *et al.* (1989). It was found that the strong condition of quasi-harmonicity resulted in a cross-correlation between gravity and surface density, which was much higher than the empirically calculated value (80–90 per cent instead of 50–60 per cent). Also, the quasi-harmonic autocovariance functions implied strong vertical and lateral density correlations. So an alternative was needed, which would enable us to model the empirically observed statistical characteristics of the density distribution and its associated external gravity field.

This alternative was found in a class of functions closely related to the base functions of blocks of constant density. The construction and use of these functions will be the main subject of this paper.

We will have to use some rather advanced, but in reality simple mathematical tools (see Moritz 1980). Most important is the equivalence between a so-called reproducing kernel and a covariance function.

For a linear vector space with inner product, $\langle\cdot,\cdot\rangle$, the reproducing kernel, $K(P, Q)$, has (if it exists) the property that

$$f(P) = \langle f(Q), K(P, Q)\rangle, \quad (2)$$

where f is an element of the space. The space will be spanned by a system of orthonormal base functions, f_i, $\langle f_i, f_j\rangle = \delta_{ij}$ and

$$K(P, Q) = \sum_{i=1}^{N} f_i(P) f_i(Q) \quad (3)$$

where N is the dimension of the space (contingently infinite). The equivalent stochastic process is spanned by all linear combinations of the stochastic variables which to a function, f, gives its coefficient a_i in the (generalized) Fourier expansion, $f = \sum_{i=1}^{N} a_i f_i$, $a_i = \langle f, f_i\rangle$. These stochastic variables will e.g. be normally distributed with variance equal to 1. The autocovariance function will be the reproducing kernel, i.e. the covariance of two values of an *arbitrary* function f, $f(P)$, $f(Q)$, will be equal to $K(P, Q)$; see Parzen (1959/1967).

2 COVARIANCE FUNCTIONS DERIVED FROM BLOCKS OF CONSTANT DENSITY

A geological structure, region, (or a profile) is in many cases described mathematically as consisting of various blocks of constant density, i.e.

$$\rho(P) = \sum_{i=1}^{N} \rho_i I_i(P), \quad (4)$$

where I_i is the so-called indicator function equal to 1 within the block and zero outside. If the blocks do not overlap, ρ_i is the density of the ith block.

The functions I_i form the base functions in a linear vector space, which will be a Hilbert space if it is equipped with the L_2 norm. If the blocks do not overlap, the functions are orthogonal, with norm equal to the square root of the volume,

$$\|I_i\|^2 = \int (I_i)^2\, dR^q = v_i; \quad (5)$$

$q = 1$, 2 or 3 depending on the dimension in which we chose to work. (We will in future suppose $q = 3$.) This Hilbert space of disjoint blocks will have a simple reproducing kernel,

$$K(P, Q) = \sum_{i=1}^{N} I_i(P) I_i(Q)/v_i, \quad (6)$$

where P, Q are both points in space. This is easily seen by inserting equations (6) and (4) into (2). This reproducing kernel may, when multiplied by an appropriate scale factor, be used as a covariance function of the density. The specific kernel given by equation (6) represents the situation where two density values are 100 per cent correlated when they are within the same block, and zero when they are in different blocks.

This covariance model is frequently used explicitly or implicitly, when solving the inverse gravimetric problem. But it is clearly physically incorrect; see Hein *et al.* (1989) or Strykowski (1989). However, we immediately see that this model gives us the possibility of using a density variance, which changes from block to block. Equation (6) shows that the density variance for a point in the ith block is equal to $1/v_i$. Hence, the variance is inversely proportional to the block size.

A simple method to create correlations between density values is to use overlapping indicator functions; see Hein *et al.* (1989). But we have to be careful as the following simple example will show.

Suppose we have two blocks, I_1, I_2, where I_1 is fully contained in I_2. In order to find the reproducing kernel, we must find the corresponding orthonormal base function, $\bar{I}_1$ *and* $\bar{I}_2$ e.g. using the Gram–Smidt procedure. Let $\langle\cdot,\cdot\rangle$ be the inner product, equal to the integral of the product of the two elements. Then

$$\bar{I}_1 = I_i/(v_1)^{1/2},$$
$$\bar{I}_2 = (I_2 - \langle \bar{I}_1, I_2\rangle \bar{I}_1)/\|I_2 - \langle \bar{I}_1, I_2\rangle I_1\|$$
$$= (I_2 - v_2 I_1/v_1)/(v_2 - v_1)^{1/2}$$
$$= (I_2 - I_1)/(v_2 - v_1)^{1/2}.$$

Hence $\bar{I}_1$ and $\bar{I}_2$ are disjoint. This small example shows that we do not get any correlations between the blocks in this case.

When the indicator functions overlap, we must first construct an equivalent set of orthonormal base functions, $\bar{I}_i$. The reproducing kernel is then (*cf.* equation 13)

$$K(P, Q) = \sum_{i=1}^{N} \bar{I}_i(P)\bar{I}_i(Q). \quad (7)$$

When scaled with an appropriate constant, σ^2, then this may be used as a covariance function. The cross-covariances between any other quantities are then obtained by applying the functionals associated with these quantities on $K(P, Q)\sigma^2$. For the autocovariance of two gravity distrubances, $\delta g(P)$, $\delta g(Q)$, the value will be equal to the product sum of the radial components of the attraction vectors produced by each function $\bar{I}_i$, evaluated at P, Q, respectively.

Because the functions $\bar{I}_i$ are linear combinations of the original functions I_i, it is easier to express and calculate the covariances using the original, presumably simpler, blocks. This can be done using the Cholesky decomposed of the matrix $\mathbf{C}$, formed by the inner products of the original blocks,

$$\langle I_i, I_j\rangle = C_{ij} = \int I_i(P)I_j(P)\, dR^3 = v_{ij} \quad (8)$$

where v_{ij} is the volume common to the two blocks. Let

$$\mathbf{C} = \mathbf{U}^{\mathrm{T}}\mathbf{U} \quad (9)$$

where $\mathbf{U}$ is upper-triangular. Then

$$\{\bar{I}_j\} = \{U_{ij}\}^{-1}\{I_i\} \quad (10)$$

is the vector of orthonormalized base functions. It is easily seen that

$$\langle \bar{I}_j, \bar{I}_i\rangle = \langle \{\mathbf{U}^{-1}\}_j\{I_m\}, \{\mathbf{U}^{-1}\}_i\{I_k\}\rangle$$
$$= \{\mathbf{U}^{-1}\}_j^{\mathrm{T}}\{\langle I_m, I_n\rangle\}\{\mathbf{U}^{-1}\}_k$$
$$= \{\mathbf{U}^{-1}\}_j^{\mathrm{T}}\mathbf{C}\{\mathbf{U}^{-1}\}_k = \delta_{jk}. \quad (11)$$

The covariance function may then be expressed in matrix form as

$$\sigma^2 K(P, Q) = \sigma^2\{I_j(P)\}^{\mathrm{T}}\mathbf{C}^{-1}\{I_k(Q)\}$$
$$= \sigma^2[\mathbf{U}^{-1}\{I_j(P)\}]^{\mathrm{T}}[\mathbf{U}^{-1}\{I_k(Q)\}]. \quad (12)$$

Let $\delta g_i(P)$, $\delta g_i(Q)$ be the radial components of the attraction vector at P, Q, respectively due to the ith block, I_i. Then

$$\mathrm{cov}\,[\delta g(P), \delta g(Q)] = \sigma^2[\mathbf{U}^{-1}\{\delta g_i(P)\}]^{\mathrm{T}}[\mathbf{U}^{-1}\{\delta g_i(Q)\}],$$

i.e. it is scalar product of the Cholesky reduced of the vectors $\{\delta g_i(P)\}$ and $\{\delta g_i(Q)\}$. This product is obtained in practice by appending the two vectors as new columns to the $\mathbf{U}$ matrix, and then continuing the Cholesky reduction by two further steps, but only making a partial reduction of the two new columns to row $N + 1$.

3 NUMERICAL INVESTIGATIONS USING RECTANGULR BLOCKS OF CONSTANT VOLUME AND DENSITY

In order to investigate numerically the properties of covariance functions created as described in Section 2, a FORTRAN program COVBLK was written. Since we wanted to study the influence of changing the block size and the overlap on the various derived covariance functions, a simple method for creating the block structure was implemented.

The block structure was specified by the following information.

(1) The (x, y, z) position of the lower, left corner of the first block.

(2) The side lengths of the blocks (supposed to be identical for all blocks), sx, sy, sz.

(3) The 'shift' dx, dy and dz to the following blocks: translations $(dx, 0, 0)$, $(0, dy, 0)$, $(0, 0, dz)$, $(dx, dy, 0)$, $(0, dy, dz)$ and (dx, dy, dz) were all applied.

(4) The number of shifts to be applied in each direction, n_x, n_y, n_z.

A structure would hence consist of totally $n_x n_y n_z$ blocks.

This algorithm had the advantage that the volumes v_{ij} were very easy to calculate, and that it was very easy to find when v_{ij} was equal to zero. Obviously, the $\mathbf{C}$ matrix, and thereby $\mathbf{U}$, will contain very many zero elements, a fact which naturally was used when computing $\mathbf{U}$.

The covariance of two density values, $\mathrm{cov}\,(P, Q)$, is then computed from $\mathbf{U}$ with two new columns appended. These columns will have elements equal to 1 if P, Q, respectively are within the block with number equal to the element number, and zero elsewhere. For 'gravimetric' quantities, the columns will have elements equal to the 'gravimetric' effects of each block, I_i. This effect was calculated using the subroutine PRISM1, written by R. Forsberg (Forsberg 1984). It allows computation of the contribution of one block to the geoid, the gravity disturbance, the gravity anomaly, the deflection of the vertical and several second-order derivatives.

Many numerical experiments were executed, but only one will be described here. The block size and number of blocks was held fixed, and the gravimetric quantities were computed at the surface of the block structure. The density functionals were evaluated just below the surface or at the depth of 1 km. The block side lengths were equal to

$$sx = sy = 10\ \mathrm{km}, \qquad sz = 1\ \mathrm{km},$$

and the numbers of shifts were

$$n_x = n_y = 8, \qquad n_z = 4.$$

Four different shifts were then applied:

(1) $dx = dy = 0.1°$, $dz = 1$ km (disjoint blocks);
(2) $dx = dy = 0.075°$, $dz = 0.75$ km;
(3) $dx = dy = 0.05°$, $dz = 0.5$ km; and
(4) $dx = dy = 0.04°$, $dz = 0.4$ km.

The results are shown in Figs 1–11 for autocovariance

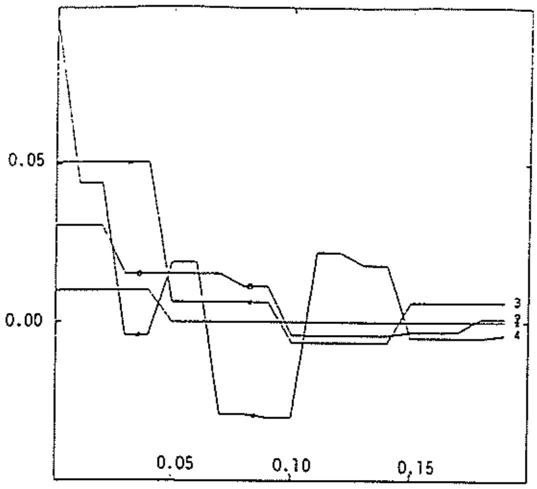

Figure 1. Density covariance at 500 m depth. Units: $(10^3\,kg\,m^{-3})^2$. ——— 1 0 per cent block overlap. —⊖— 2 25 per cent block overlap. —×— 3 50 per cent block overlap. —●— 4 60 per cent block overlap. The legend is the same for all figures. In all figures the horizontal scale (x axis) shows the distance from the first point in degrees.

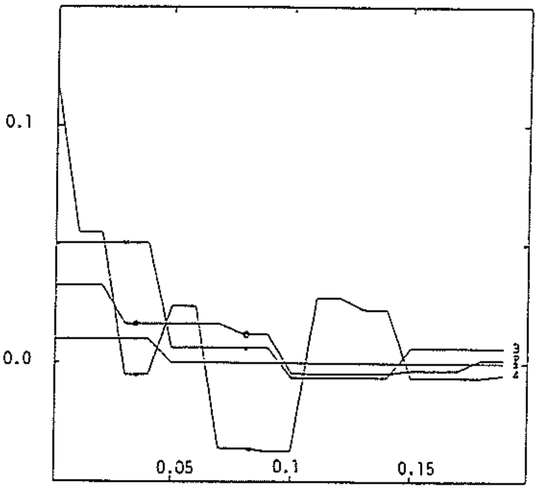

Figure 2. Density covariance function at 1000 m depth. Units: $(10^3\,kg\,m^{-3})^2$.

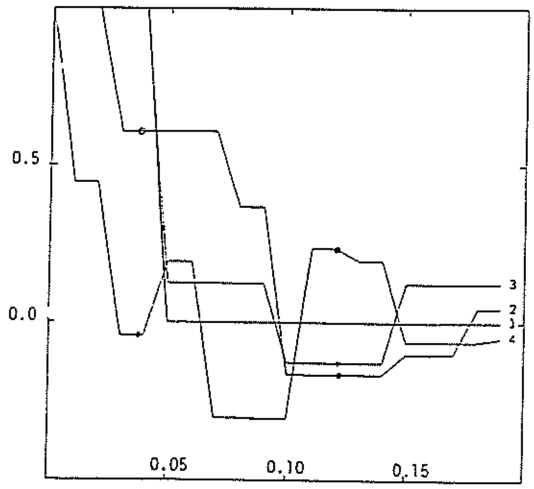

Figure 3. Density correlation function (depth independent).

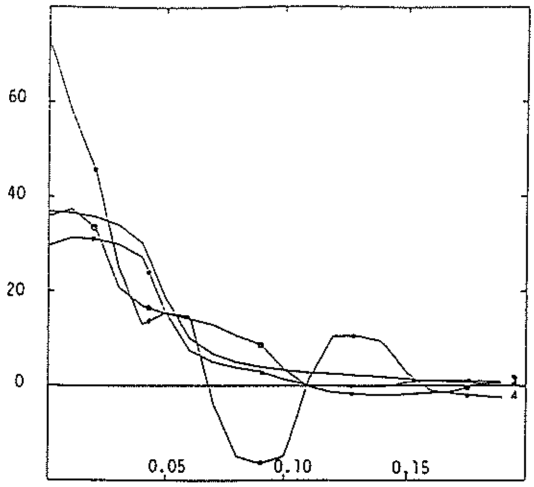

Figure 4. Gravity disturbance covariance. Function in units of $(10^{-5}\,m\,s^{-2})^2$.

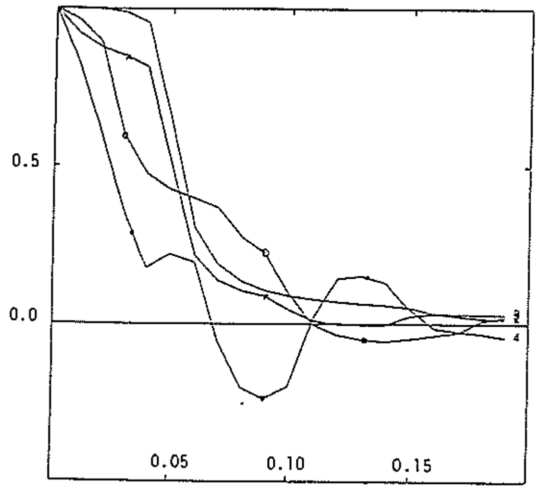

Figure 5. Gravity disturbance correlation function with first point at a fixed point.

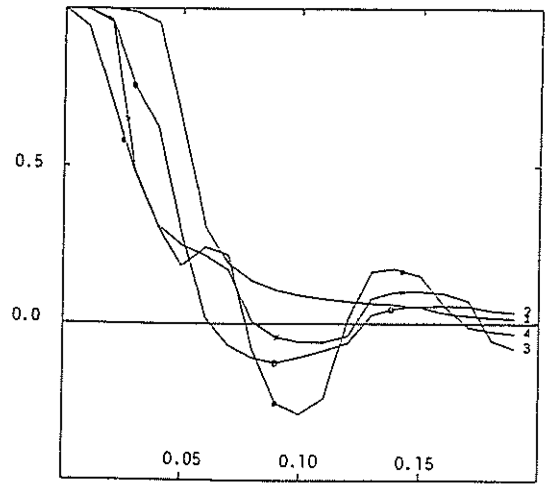

Figure 6. Gravity disturbance correlation function, with first point at the middle of a block.

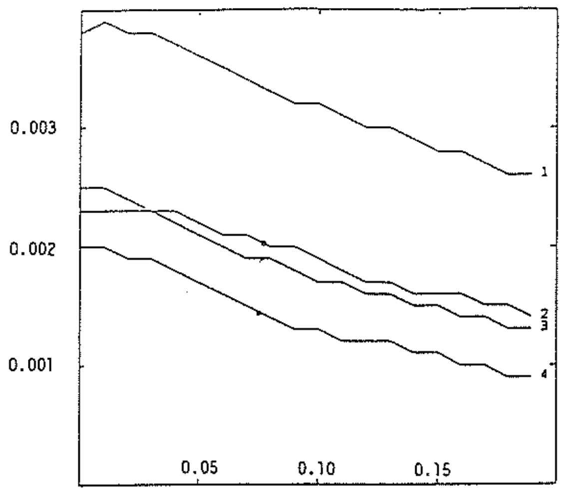

Figure 7. Geoid covariance function (m^2).

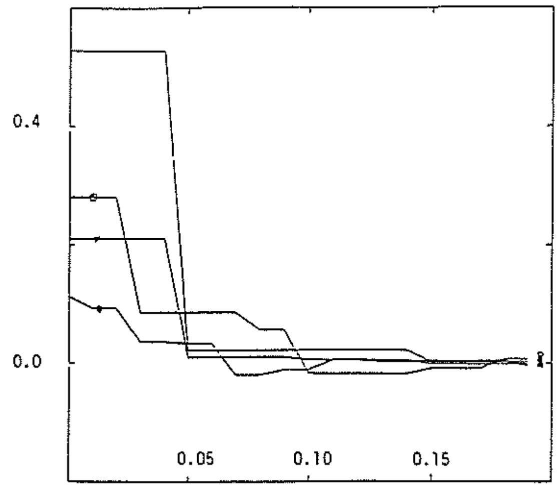

Figure 10. Correlation function between surface gravity disturbance and density at 1 km depth.

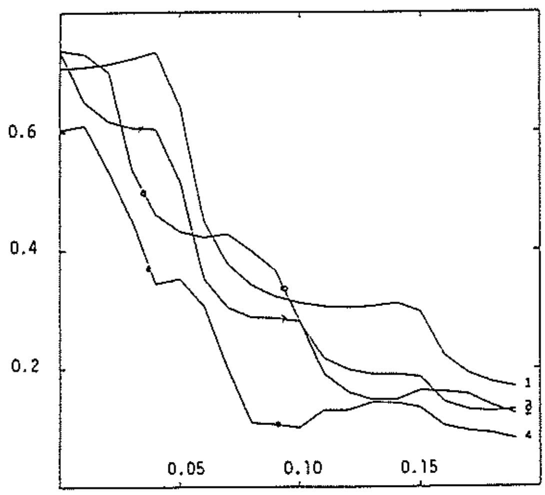

Figure 8. Correlation function gravity disturbance-geoid.

functions of density, gravity disturbance, and geoid, and cross-*correlation* functions for the combined quantities. (A block density of 100 $kg\,m^{-3}$ was used in all cases).

The covariance functions were computed between a fixed point, P, and points Q_i, $i = 0, \ldots, 19$, Q_i having the same (x, y) coordinates as P, but then being shifted $0.01° \approx 1$ km in x for each i.

For the reader who is familiar with empirical covariance functions derived from gravimetric quantities (see e.g. Knudsen 1987; Hein *et al.* 1989), it will be clear from inspection of Figs 4–8, that the functions look very much like those found in practice. The most striking difference as compared to known functions, is the constant values found for the auto- and cross-correlation functions with density anomalies. However, this phenomenon is caused by the fact that when the point Q_i changes, it may not simultaneously jump to a new block!

For the density (auto) covariance functions, a zero point (but not necessarily the very first) occurs at a distance corresponding to the basic block size, while the correlation distance depends on the overlap. The larger the overlap,

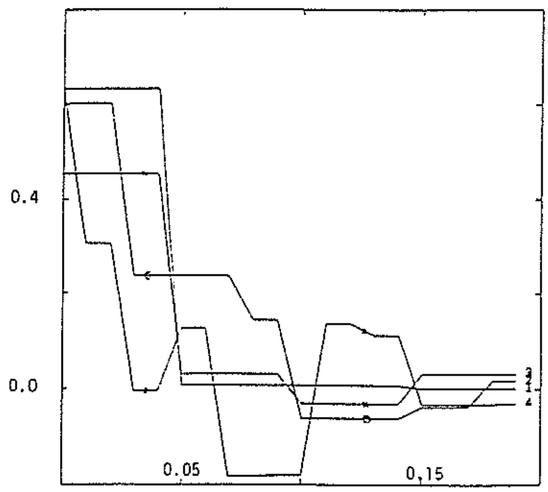

Figure 9. Correlation function, surface gravity disturbance and density.

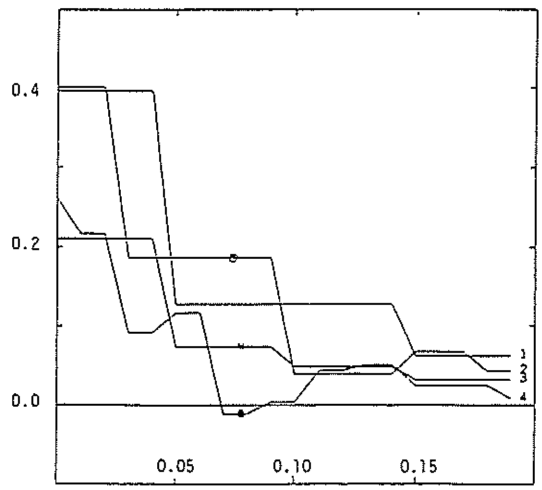

Figure 11. Correlation function, geoid and surface density.

then *in general* the shorter the correlation distance (see Figs 5 and 6). It has not been possible to establish a general rule, possibly due to the phenomenon described in Section 2, which occurs when one block is fully within another. This phenomenon also seems to occur when blocks fit exactly together, as when a 50 per cent overlap is used.

An important result is seen when inspecting Fig. 9, which shows the cross-correlation function between surface gravity and density. The correlations for zero spherical distance are within the interval 0.4–0.7. This means that it is possible to model the empirically observed correlation found in Hein *et al.* (1989).

4 APPLICATION OF THE COVARIANCE MODELS

Covariance functions produced by overlapping blocks of constant density provide a flexible tool for the realistic modelling of empirical auto- and cross-covariance functions. A variation of the block size will permit the modelling of a situation where the density variance changes laterally or with depth. A change of the size of the blocks and the block overlap produce gravity covariance functions with changing correlation distance and location of the first zero-point. Consequently, the shape of an empirical auto-covariance function of gravity may be used to select block size and overlap.

When used to solve the inverse gravimetric problem, error estimates of point density values may be computed. This may be used in simulation studies in order to investigate how well density values may be estimated using varying data configurations, and the dependence of the result on the parametrization of the geological structure.

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