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COVARIANCE FUNCTIONS IN LEAST-SQUARES COLLOCATION

by
Helmut Moritz

The Ohio State University
Department of Geodetic Science
1958 Neil Avenue
Columbus, Ohio 43210

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ABSTRACT

The report consists of two parts. Part A deals with the mathematical structure of covariance functions. The properties of isotropy, harmonicity and positive definiteness are discussed, and it is suggested that a covariance function may be characterized by three essential parameters: the variance, the correlation length and a curvature parameter. Finally some spatial covariance models (planar and spherical) are considered.

Part B treats the influence of covariances on the results of collocation. Formulas are developed for the standard error of collocation results when using non-optimal covariance functions, also for the case of stepwise collocation. Finally the behavior of interpolation errors with and without the additional use of horizontal gradients is studied by means of power series expansions for covariance functions and by means of Gaussian covariance functions. It is seen that non-optimal covariance functions have relatively little influence on the interpolated values but a very strong effect on covariances as calculated using the conventional formulas.

FOREWORD

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CONTENTS

INTRODUCTION

Least-squares collocation depends essentially on the covariance functions used. This is especially true for accuracy studies, for which, on the other hand, collocation provides a powerful mathematical apparatus.

For instance, it is known that some analytical expressions for covariance functions lead to imaginary standard errors. What is wrong with such functions? They are not positive definite.

It is also well known that the covariance functions are responsible for the precise mathematical structure of the gravity field through covariance propagation. This implies that the basic covariance functions must be harmonic.

It appears, therefore, appropriate to elaborate, in some details, mathematical properties of covariance functions such as positive definiteness and harmonicity.

Another question is how to characterize a covariance function sufficiently well by a small number of parameters, in such a way that two different covariance functions that have these parameters in common, give approximately the same result.

To find a good analytical covariance function, one tries to represent it as a linear combination of simpler functions. It is, therefore, desirable to know ~~th~~e behavior of such simple models which may serve as building blocks for a global covariance function.

All these problems will be considered in the first part of the report. The second part deals with the following question: What happens if the "true" covariance function is unknown and least-squares collocation is, instead, performed with a "wrong" (or more precisely, non-optimal) covariance function?

How does the result change with respect to the optimal case, and what is the effect on accuracy studies? General formulas will be developed and applied to simple interpolation problems. The numerical results so obtained, special as they are, may nevertheless give some indication as to what can happen in more general situations. At any rate, the mathematical apparatus is now available to attack also problems of greater complexity.

PART A

ON THE MATHEMATICAL STRUCTURE OF COVARIANCE FUNCTIONS

1. Isotropy and Harmonicity

A rotationally symmetric spatial covariance function has the form (Moritz, 1972, sec.7)

$$K(P,Q) = \sum_{n=o}^{\infty} k_n \left(\frac{R^2}{r_P r_Q}\right)^{n+1} P_n(\cos\psi) \ , \qquad (1\text{-}1)$$

where P and Q are two points in space, of radius vectors r_P and r_Q , ψ is the angle between r_P and r_Q , $R = 6370$ km is the mean radius of the earth, the $P_n(\cos\psi)$ are the Legendre polynomials, and k_n are positive coefficients.

Since the function depends only on ψ , the spherical distance between the points P and Q , it is rotationally symmetric (invariant with respect to the three-dimensional rotation group), that is, isotropic and homogeneous on the sphere.

The dependence on r_P and r_Q is such that any $K(P,Q)$ of this form will be harmonic, that is, will satisfy Laplace's equation, with respect to both points P and Q . This is necessary if $K(P,Q)$ is to be the covariance function of the anomalous gravitational potential T , which is supposed to be harmonic outside the sphere $r = R$.

Hence $K(P,Q)$, which is a priori a function of six variables, namely of the three coordinates of both P and Q , reduces in view of symmetry and harmonicity to a function of two essential variables, namely ψ and the product $r_P r_Q$:

$$K(P,Q) = F(\psi, r_P r_Q) = \sum_{n=0}^{\infty} k_n P_n(\cos\psi) \ . \tag{1-2}$$

It is clear that on the surface of the terrestrial sphere $r = R$, that is, for $r_P = r_Q = R$, the function (1-1) reduces to a function of ψ only:

$$K(P,Q) = \sum_{n=0}^{\infty} k_n P_n(\cos\psi) \ . \tag{1-3}$$

For local applications it is frequently convenient to use a planar approximation, replacing the surface of the terrestrial sphere locally by a plane, which will be taken as the xy-plane $(z=0)$ of a local cartesian coordinate system. Then, on this plane, a stationary and isotropic covariance function will be a function only of the distance

$$s = \sqrt{(x_P - x_Q)^2 + (y_P - y_Q)^2} \tag{1-4}$$

between points P and Q :

$$K(P,Q) = K(s) \ . \tag{1-5}$$

On introducing the "Hankel transform" of this function by

$$G(n) = \frac{1}{2\pi} \int_0^{\infty} J_o(ns) K(s) s\,ds \ , \tag{1-6}$$

where $J_o(x)$ is the Bessel function of zero order, we may express $K(s)$ in the form

$$K(s) = 2\pi \int_0^{\infty} J_o(ns) G(n) n\,dn \ . \tag{1-7}$$

This is a consequence of homogeneity and isotropy; cf. (Bartlett, 1960, p.192; Papoulis, 1968, p.142).

To extend the function $K(s)$, defined for $z = 0$, into upper half space $z \geqq 0$ (corresponding to outer space), we use the harmonicity of $K(P,Q)$, considered as a function of <u>spatial</u> points P and Q. We shall try an expression of the form

$$K(P,Q) = 2\pi\int_0^\infty J_0(\eta s)G(\eta)\phi(z_P,\eta)\phi(z_Q,\eta)\eta d\eta . \tag{1-8}$$

This expression may be motivated by the analogy between the spectral representations (1-2) and (1-7). There correspond:

ψ to s,
integral to sum,
variable η to index n,
$J_0(\eta s)$ to $P_n(\cos\psi)$,
$G(\eta)$ to c_n.

Therefore, it is evident to expect that some factor $\phi(z_P,\eta)$ will correspond to the factor $(R/r_P)^{n+1}$. The functions $\phi(z_P,\eta)$ and $\phi(z_Q,\eta)$ must have the same form because of symmetry.

In cylindric coordinates s,α,z, Laplace's equation may be written:

$$\Delta f = f_{ss} + \frac{1}{s}f_s + \frac{1}{s^2}f_{\alpha\alpha} + f_{zz} = 0 ; \tag{1-9}$$

for rotationally symmetric functions which do not depend on the azimuth α, this reduces to

$$f_{ss} + \frac{1}{s}f_s + f_{zz} = 0 . \tag{1-10}$$

Since the spatial function

$$K(P,Q) = K(s,z_1,z_2) \tag{1-11}$$

must satisfy this equation both at P and at Q, we must have

$$\frac{\partial^2 K}{\partial s^2} + \frac{1}{s}\frac{\partial K}{\partial s} + \frac{\partial^2 K}{\partial z_P^{\,2}} = 0 , \tag{1-12}$$

$$\frac{\partial^2 K}{\partial s^2} + \frac{1}{s}\frac{\partial K}{\partial s} + \frac{\partial^2 K}{\partial z_Q^2} = 0 . \tag{1-13}$$

Using the representation (1-8) with (1-12) gives the condition

$$\left[\frac{\partial^2 J_o(ns)}{\partial s^2} + \frac{1}{s}\frac{\partial J_o(ns)}{\partial s}\right]\phi(z_P,n) + J_o(ns)\frac{\partial^2\phi(z_P,n)}{\partial z_P^2} = 0 . \tag{1-14}$$

Since the Bessel function $y = J_o(x)$ satisfies the well-known differential equation

$$y'' + \frac{1}{x}y' + y = 0 , \tag{1-15}$$

we have

$$\frac{\partial^2 J_o(ns)}{\partial s^2} + \frac{1}{s}\frac{\partial J_o(ns)}{\partial s} = -n^2 J_o(ns) ,$$

so that (1-14) reduces to

$$\frac{\partial^2\phi(z_P,n)}{\partial z_P^2} - n^2\phi(z_P,n) = 0 \tag{1-16}$$

with solution

$$\phi(z_P,n) = e^{-nz_P} \tag{1-17}$$

satisfying the required boundary conditions

$$\phi = 1 \quad \text{if} \quad z = 0 \,, \qquad \phi \to 0 \quad \text{if} \quad z \to \infty \,. \tag{1-18}$$

Likewise we have

$$\phi(z_Q,n) = e^{-nz_Q}, \tag{1-19}$$

so that (1-8) becomes

$$K(P,Q) = 2\pi\int_0^\infty J_o(ns)G(n)e^{-n(z_P+z_Q)}\,ndn \,. \tag{1-20}$$

We thus have obtained the essential result that the elevations z_P and z_Q enter in $K(P,Q)$ only through their sum $z_P + z_Q$, so that we have

$$K(P,Q) = F(s,z_P+z_Q) \,. \tag{1-21}$$

This form, which is valid for plane symmetry (homogeneity and isotropy in the xy-plane) is obviously the analogue of (1-2), which holds for spherical symmetry.

<u>Consequences for the Covariances of Gradients</u>.- From the form (1-21) we may derive, in a simple way, important consequences for the covariances of first-order gradients T_x, T_y, T_z .

The covariances of these gradients are readily expressed in terms of $K(P,Q)$ by covariance propagation

(Moritz, 1972, sec.7). We have

$$\operatorname{cov}(T_{x,P}, T_{x,Q}) = \frac{\partial^2 K}{\partial x_P \partial x_Q} \quad , \tag{1-22a}$$

$$\operatorname{cov}(T_{y,P}, T_{y,Q}) = \frac{\partial^2 K}{\partial y_P \partial y_Q} \quad , \tag{1-22b}$$

$$\operatorname{cov}(T_{z,P}, T_{z,Q}) = \frac{\partial^2 K}{\partial z_P \partial z_Q} \quad . \tag{1-22c}$$

Write now (1-21) in the form

$$K(P,Q) = F(s,Z) \tag{1-23}$$

where

$$Z = z_P + z_Q \ . \tag{1-24}$$

Differentiating (1-4) gives

$$\frac{\partial s}{\partial x_P} = - \frac{x_Q - x_P}{s} = - \frac{\partial s}{\partial x_Q} \quad , \tag{1-25}$$

so that

$$\frac{\partial K}{\partial x_P} = - \frac{\partial F}{\partial s} \frac{x_Q - x_P}{s} \quad ,$$

$$\frac{\partial^2 K}{\partial x_P^2} = \frac{1}{s} \frac{\partial F}{\partial s} + \frac{1}{s} \frac{\partial}{\partial s}\left(\frac{1}{s} \frac{\partial F}{\partial s}\right)(x_Q - x_P)^2 = - \frac{\partial^2 K}{\partial x_P \partial x_Q} \quad . \tag{1-26}$$

In the same way one shows that

$$\frac{\partial^2 K}{\partial y_P^2} = \frac{1}{s} \frac{\partial F}{\partial s} + \frac{1}{s} \frac{\partial}{\partial s}\left(\frac{1}{s} \frac{\partial F}{\partial s}\right)(y_Q - y_P)^2 = - \frac{\partial^2 K}{\partial y_P \partial y_Q} \quad . \tag{1-27}$$

We further have by (1-24)

$$\frac{\partial K}{\partial z_P} = \frac{\partial F}{\partial Z} ,$$

$$\frac{\partial^2 K}{\partial z_P^2} = \frac{\partial^2 F}{\partial Z^2} = \frac{\partial^2 K}{\partial z_P \partial z_Q} . \tag{1-28}$$

Thus Laplace's equation

$$\frac{\partial^2 K}{\partial x_P^2} + \frac{\partial^2 K}{\partial y_P^2} + \frac{\partial^2 K}{\partial z_P^2} = 0$$

gives immediately

$$\frac{\partial^2 K}{\partial z_P \partial z_Q} = \frac{\partial^2 K}{\partial x_P \partial x_Q} + \frac{\partial^2 K}{\partial y_P \partial y_Q} , \tag{1-29}$$

which provides an important relation between the covariance functions of the first-order gradients T_x, T_y, T_z . This relation, which may be used for checking and other purposes, is all the more remarkable as a similar relation between the first-order gradients themselves does not exist. It exists only for second-order gradients:

$$T_{zz} = -(T_{xx}+T_{yy}) . \tag{1-30}$$

The relation (1-29) expresses, essentially, the covariance function of the gravity anomalies ($\Delta g=T_z$) as the sum of the autocovariance functions of the components of the deflection of the vertical ξ, η (which are proportional to T_x and T_y). This may be rather surprising.

As a matter of fact, the covariance function of T_z, given by (1-22c), has also the structure $F(s,Z)$, being a function only of s and Z. From this we conclude that, e.g., the covariance function of the second-order gradient T_{zz} is the sum of the auto-covariance functions of the gradients T_{xz} and T_{yz}, and so on for higher gradients.

It should, however, be mentioned that mixed covariances, e.g. between T_x and T_z, cannot be obtained in this way.

By adding (1-26) and (1-27) we get from (1-29)

$$\frac{\partial^2 K}{\partial z_P \partial z_Q} = -\frac{2}{s}\frac{\partial F}{\partial s} - s\frac{\partial}{\partial s}\left(\frac{1}{s}\frac{\partial F}{\partial s}\right)$$

$$= -\frac{1}{s}\frac{\partial F}{\partial s} - \frac{\partial^2 F}{\partial s^2} .$$

In the plane $z = 0$ we, therefore, have for $K(P,Q) = K(s)$:

$$\frac{\partial^2 K}{\partial z_P \partial z_Q} = - K''(s) - \frac{1}{s}K'(s) . \tag{1-31}$$

This relation expresses the covariance function of the vertical derivative $\partial T/\partial x$ in terms of horizontal derivatives of the covariance function.

Let us similarly calculate the covariance function of the horizontal components. If we assume that P and Q are both situated on the x-axis, then

$$x_Q - x_P = s , \qquad y_Q - y_P = 0 , \tag{1-32}$$

and (1-26) and (1-27) give

$$\frac{\partial^2 K}{\partial x_P \partial x_Q} = -\frac{1}{s}\frac{\partial F}{\partial s} - s\frac{\partial}{\partial s}\left(\frac{1}{s}\frac{\partial F}{\partial s}\right) ,$$

$$\frac{\partial^2 K}{\partial y_P \partial y_Q} = -\frac{1}{s}\frac{\partial F}{\partial s} .$$

For $z = 0$ and $F(s,0) = K(s)$ this becomes

$$\frac{\partial^2 K}{\partial x_P \partial x_Q} = -K''(s) , \tag{1-33}$$

$$\frac{\partial^2 K}{\partial y_P \partial y_Q} = -\frac{1}{s}K'(s) . \tag{1-34}$$

These are the longitudinal and transversal covariances; cf. (Grafarend, 1971) and (Moritz, 1972, pp.109-113).

These expressions relate the autocovariance functions of gravity anomalies and of vertical deflections; they may be taken into account for an optimal determination of the covariance function from different kinds of data.

2. Positive Definiteness

Consider the signals $s_1, s_2, \ldots, s_m$ at an arbitrary number m of points; these signals may, for instance, be the values of the anomalous potential T at these points. Form their linear combination

$$u = \lambda_1 s_1 + \lambda_2 s_2 + \ldots + \lambda_m s_m = \sum_{i=1}^{m} \lambda_i s_i \, , \tag{2-1}$$

where the λ_i are arbitrary constant coefficients. The variance of the random variable u is (M denotes the statistical expectation):

$$M\{u^2\} = \sum_{i=1}^{m} \sum_{j=1}^{m} \lambda_i \lambda_j M\{s_i s_j\} = \sum_{i=1}^{m} \sum_{j=1}^{m} C_{ij} \lambda_i \lambda_j \, , \tag{2-2}$$

where

$$C_{ij} = M\{s_i s_j\} \tag{2-3}$$

denotes the signal covariances. Since

$$M\{u^2\} \geqq 0 \, , \tag{2-4}$$

we must have the basic condition

$$\sum_{i=1}^{m} \sum_{j=1}^{m} C_{ij} \lambda_i \lambda_j \geqq 0 \, , \tag{2-5}$$

which expresses the fact that covariance matrices must be <u>positive definite</u>[1).

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1) Positive definiteness in the strict sense corresponds to the $>$ sign in (2-5) only, excluding the equality sign. Hence it would be more precise to speak of positive semidefiniteness, but we shall use the shorter name.

In the case of a continuous signal field s , the covariances can be derived from a covariance function $K(P,Q)$ by

$$C_{ij} = K(P_i, P_j) \ . \tag{2-6}$$

This gives a fundamental condition for the covariance function:

$$\sum_{i=1}^{m} \sum_{j=1}^{m} K(P_i, P_j) \lambda_i \lambda_j \geqq 0 \ , \tag{2-7}$$

which it must satisfy for arbitrary points P_i and arbitrary constants λ_i . Functions satisfying (2-7) are called <u>positive definite</u>.

Positive definite functions can be mathematically characterized as functions which have a spectrum which is everywhere positive (more precisely, nonnegative). For the representation (1-1) this means that the coefficients k_n are never negative:

$$k_n \geqq 0 \quad \text{for all} \quad n \ . \tag{2-8}$$

In the planar case (1-20) the spectrum is the <u>Hankel transform</u> $G(\eta)$, so that the corresponding condition reads

$$G(\eta) \geqq 0 \quad \text{for all} \quad \eta \geqq 0 \ , \tag{2-9}$$

where $G(\eta)$ is given by (1-6).

A simpler condition is obtained by considering only points P_i lying on an arbitrary straight line in the horizontal plane $z = 0$; without loss of generality we may consider this straight line as the x-axis . Then the spectrum is the Fourier transform

$$S(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega x} C(x)\,dx \ , \tag{2-10}$$

so that the condition for positive definiteness becomes

$$S(\omega) \geqq 0 \ . \tag{2-11}$$

The condition (2-8) is necessary and sufficient for isotropic covariance functions on the sphere. Since such functions (1-3) have a unique harmonic extension (1-1) into outer space, (2-8) is necessary and sufficient for isotropic and harmonic covariance functions in space.

For similar reasons, (2-9) is necessary and sufficient for spatial covariance functions homogeneous and isotropic in the plane $z = 0$ and harmonic for $z \geqq 0$ (provided the spectrum is continuous, that is, the integral (1-6) exists).

All isotropic and homogeneous covariance functions in the plane $z = 0$ are also homogeneous on the x-axis only; therefore all covariance functions having positive Hankel transforms (1-6) will also have positive Fourier transforms (2-10) (provided both integrals exist). The author does not know whether the converse is also true, that is, whether (2-11) is already sufficient to guarantee positive definiteness in the plane $z = 0$ and in space $z \geqq 0$; however, if the integral (2-10) exists, the condition (2-11) is certainly necessary for planar covariance functions.

Analytic Covariance Functions.- Functions that are harmonic in a certain region, are analytic there. This justifies the consideration of analytic covariance functions.

Stationary and isotropic covariance functions analytic in the plane $z = 0$ can be expanded as power series:

$$K(s) = a_o - a_1 s^2 + a_2 s^4 - a_3 s^6 +- \dots$$
$$= \sum_{k=o}^{\infty} (-1)^k a_k s^{2k} \; . \qquad (2\text{-}12)$$

There are only even powers of s because of symmetry, and the series converges for sufficiently small s .

A necessary condition for positive definiteness is that the determinant of the covariances in (2-7) is non-negative. For $m = 3$ we thus have

$$\begin{vmatrix} K(P_1,P_1) & K(P_1,P_2) & K(P_1,P_3) \\ K(P_1,P_2) & K(P_2,P_2) & K(P_2,P_3) \\ K(P_1,P_3) & K(P_2,P_3) & K(P_3,P_3) \end{vmatrix} \geqq 0 \; . \qquad (2\text{-}13)$$

If the points P_1, P_2, P_3 lie, in the plane $z = 0$, on a straight line such that $P_1P_2 = P_2P_3 = s$, we thus have (Bartlett, 1960, p.161)

$$\begin{vmatrix} K(0) & K(s) & K(2s) \\ K(s) & K(0) & K(s) \\ K(2s) & K(s) & K(0) \end{vmatrix} \geqq 0 \; .$$

By expanding the determinant we obtain

$$\left[K(0) - K(2s)\right]\left[K^2(0) - 2K^2(s) + K(0)K(2s)\right] \geqq 0$$

or, since $K(0) - K(2s) > 0$,

$$K^2(0) - 2K^2(s) + K(0)K(2s) \geqq 0 \; , \qquad (2\text{-}14)$$

Inserting the power series (2-12) we obtain

$$(12a_o a_2 - 2a_1^2)s^4 + O(s^6) \geqq 0 \;,$$

or dividing by $2s^4$ and letting $s \to 0$,

$$6a_o a_2 - a_1^2 \geqq 0 \;. \tag{2-15}$$

This is a relation linking the first three coefficients of the series (2-12). To get relations between the following coefficients, we note that by (1-33) the function

$$- K''(s) = 2a_1 - 12a_2 s^2 + 30a_3 s^4 - + \ldots \tag{2-16}$$

is also a covariance function, namely for the horizontal gradient $\partial T/\partial x$. For this series, the relation corresponding to (2-15) is

$$6(2a_1)(30a_3) - (12a_2)^2 \geqq 0$$

or

$$5a_1 a_3 - 2a_2^2 \geqq 0 \;. \tag{2-17}$$

In this way we may proceed by successive differentiation and by writing the condition (2-15) for the series

$$K^{IV}(x) \;, \quad - K^{VI}(x) \;, \quad K^{VIII}(x) \;, \text{ etc.}$$

This can be done in a general way. For the 2n - th derivative $K^{(2n)}(s)$ of the series (2-12) we have

$$(-1)^n K^{(2n)}(s) = \sum_{k=o}^{\infty} (-1)^k b_k s^{2k} \;, \tag{2-18}$$

where

$$b_k = (2k+1)(2k+2)\ \ldots(2k+2n)a_{k+n}\ . \tag{2-19}$$

Writing the condition (2-15) for the new series,

$$6b_o b_2 - b_1^2 \geqq 0\ ,$$

gives readily

$$a_{n+2} \geqq \frac{(2n+1)(2n+2)}{(2n+3)(2n+4)} \frac{a_{n+1}^2}{a_n}\ . \tag{2-20}$$

This is the basic general condition which the coefficients of the series (2-12) must satisfy. Obviously, (2-15) and (2-17) are special cases of (2-20) for $n = 0$ and $n = 1$.

<u>Examples</u>.- We shall now illustrate the general developments by means of some analytical expressions for covariance functions found in the literature. We shall write $C(s)$ instead of $K(s)$, since the functions are used as covariance functions for gravity anomalies Δg rather than for the anomalous potential T; this notation follows (Moritz, 1972, sec.7).

Let us start with <u>Hirvonen's covariance function</u> (Hirvonen, 1962; Heiskanen and Moritz, 1967, p.255):

$$C(s) = \frac{C_o}{1 + (s/d)^2} \tag{2-21}$$

with empirical constants

$$C_o = 337\ \text{mgal}^2\ , \quad d = 40\ \text{km}\ . \tag{2-22}$$

By a suitable choice of units we may put

$$C_o = 1 , \quad d = 1 ,$$

so that this function becomes

$$C(s) = \frac{1}{1 + s^2} \tag{2-23}$$

with series expansion

$$C(s) = 1 - s^2 + s^4 - s^6 + - \ldots . \tag{2-24}$$

Here all $a_n = 1$, so that (2-20) becomes

$$1 \geqq \frac{(2n+1)(2n+2)}{(2n+3)(2n+4)} ,$$

which is clearly satisfied for all n .

The Fourier transform (2-10) of (2-23) is

$$S(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\cos\omega x}{1+x^2} dx = \frac{1}{2} e^{-|\omega|} \tag{2-25}$$

(Papoulis, 1968, p.66), which is always positive. Thus Hirvonen's covariance function is, in fact, positive definite.

Consider next the <u>Gaussian function</u>

$$C(s) = C_o e^{-A^2 s^2} , \tag{2-26}$$

which has also been frequently suggested as covariance function. We again simplify by putting

$C_o = 1$, $A = 1$,

so that we have

$$C(s) = e^{-s^2} = 1 - \frac{s^2}{1!} + \frac{s^4}{2!} - \frac{s^6}{3!} + - \dots , \tag{2-27}$$

and hence $a_n = 1/n!$. Now (2-20) becomes

$$1 \geqq \frac{2n+1}{2n+3} ,$$

which is also satisfied by all n . The positive definiteness of this function is further confirmed by its Fourier transform

$$S(\omega) = \frac{1}{2\sqrt{\pi}} e^{-\omega^2/4} \tag{2-28}$$

and its Hankel transform (1-6) (Papoulis, 1968, p.145),

$$G(n) = \frac{1}{2\pi} \int_0^\infty J_o(ns) e^{-s^2} s ds = \frac{1}{4\pi} e^{-n^2/4} . \tag{2-29}$$

We finally ask whether there are functions for which the condition (2-20) is satisfied with an equality sign. This will obviously constitute some kind of limiting case. Thus the condition is

$$a_{n+2} = \frac{(2n+1)(2n+2)}{(2n+3)(2n+4)} \frac{a_{n+1}^2}{a_n} . \tag{2-30}$$

For $n = 0$ this gives

$$a_2 = \frac{1.2}{3.4}\frac{a_1^2}{a_o} = \frac{2^2}{4!}B^2A ,$$

if we set $a_o = A$, $a_1 = AB$. For $n = 1$ we obtain

$$a_3 = \frac{3.4}{5.6}\frac{a_2^2}{a_1} = \frac{2^3}{6!}B^3A ,$$

and so forth. Generally we find

$$a_n = \frac{(2B)^n}{(2n)!}A , \tag{2-31}$$

which is readily seen to satisfy (2-30).

Thus the solution to our problem is the series

$$C(s) = A\left[1 - \frac{2Bs^2}{2!} + \frac{(2B)^2s^4}{4!} - \frac{(2B)^3s^6}{6!} + - \right] , \tag{2-32}$$

the sum of which is

$$C(s) = A\cos s\sqrt{2B} . \tag{2-33}$$

Putting

$$A = C_o , \quad \sqrt{2B} = \beta , \tag{2-34}$$

we finally obtain

$$C(s) = C_o\cos\beta s , \tag{2-35}$$

which is simply the <u>cosine function</u> with two free parameters C_o and β . This is the desired limiting case for a positive-definite covariance function.

The cosine function is a limiting case also in the sense that it oscillates between the extrema C_o and $-C_o$, so that there are points $s \neq 0$ where $|C(s)| = C_o$, that is, where the covariance equals the variance. This implies the gratest possible degree of correlation, which is clearly unrealistic; for a realistic covariance function, there should be always

$$|C(s)| < C_o \tag{2-36}$$

for $s \neq 0$.

That the case $|C(s)| > C_o$ is excluded, follows again from positive definiteness: writing for $C(s)$ a condition analogous to (2-13), but for $m = 2$, we have

$$\begin{vmatrix} C(0) & C(s) \\ C(s) & C(0) \end{vmatrix} \geqq 0 , \tag{2-37}$$

from which (2-36) follows immediately.

There is a fundamental relationship between positive definiteness and predition error. For instance, consider the interpolation problem of sec. 7 (Fig. 7-1) when using Δg_1 and Δg_2 only. Then (7-20), with $K = C$, together with (7-19), gives

$$m^2_{P,1} = C_o - \frac{C^2_{Pu}}{C_{uu}} = C(0) - \frac{2C^2(a)}{C(0)+C(2a)}$$

$$= \frac{C^2(0)-2C^2(a)+C(0)C(2a)}{C(0)+C(2a)} , \tag{2-38}$$

which is positive if and only if (2-14) is satisfied.

For the cosine covariance function (2-35), $m^2_{P,1}$ is zero. This shows that there are covariance function which give zero prediction error. Hence, <u>the smallness of prediction error is by no means a criterium for a good covariance function!</u>

3. Essential Parameters for Covariance Functions

The question arises whether covariance functions can be satisfactorily characterized by means of a few parameters only. We shall give a set of three such essential parameters: the variance C_o , the "correlation length" (in German: Halbwertsbreite) ξ , and the "curvature parameter" χ ; again we shall denote the covariance function by $C(s)$ rather than by $K(s)$.

The geometrical interpretation of these quantities is simple (Fig. 3-1). The variance C_o is the value of the covariance function $C(s)$ for the argument $s = 0$:

$$C(0) = C_o \quad . \tag{3-1}$$

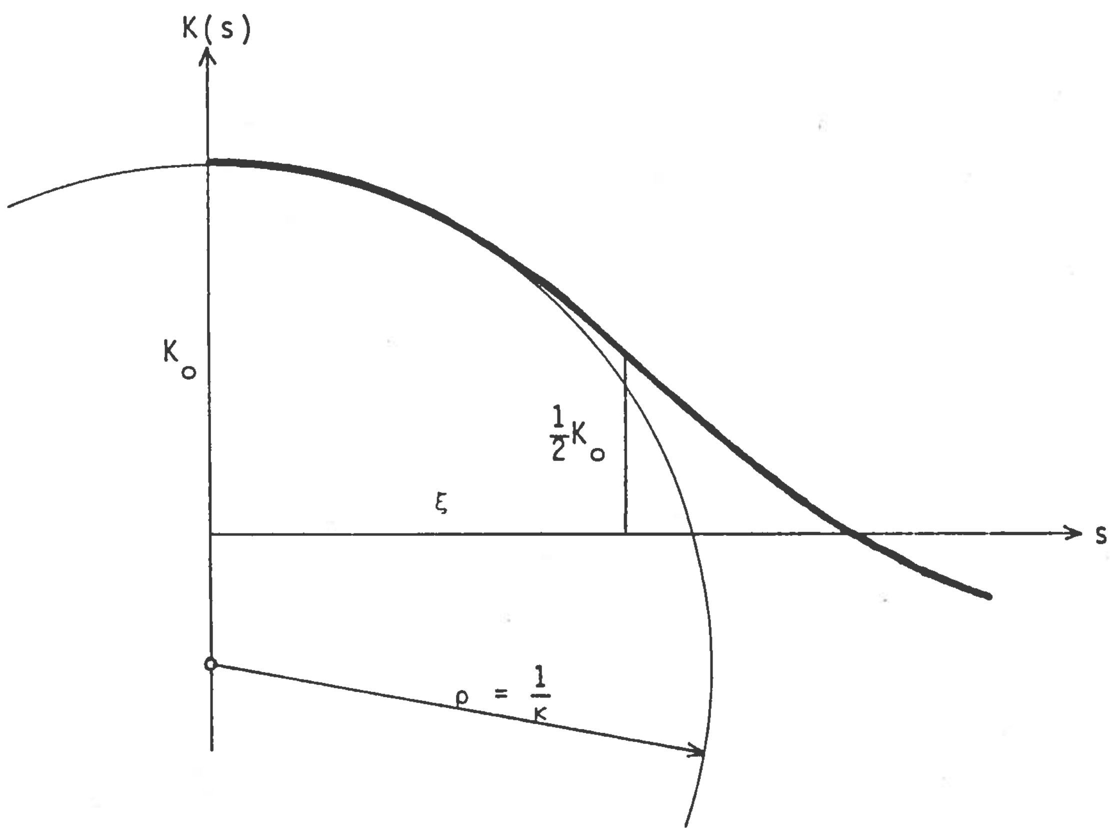

Figure 3-1

The correlation length ξ is the value of the argument for which $C(s)$ has decreased to half of its value at $s = 0$, that is

$$C(\xi) = \tfrac{1}{2}C_o \ . \tag{3-2}$$

The curvature parameter χ is a dimensionless quantity related to the curvature κ of the covariance curve at $s = 0$ by

$$\chi = \kappa\xi^2/C_o \ . \tag{3-3}$$

It can be easily expressed in terms of the coefficient a_1 of the series expansion (2-12). The well-known formula for the curvature κ,

$$\kappa = \frac{y''}{(1+y'^2)^{3/2}} \ , \tag{3-4}$$

gives for $x = s$ and $y = C(s)$ at $s = 0$:

$$\kappa = 2a_1 \ . \tag{3-5}$$

Here we have changed the sign which is irrelevant since the sign in (3-4) is conventional. Fig. 3-1 shows the radius of curvature ρ related to κ by $\rho = 1/\kappa$. From (3-3) and (3-5) we get

$$\chi = 2a_1\xi^2/C_o \ . \tag{3-6}$$

It is frequently convenient to norm the covariance function under consideration by putting

$$C_o = 1 \ , \quad \xi = 1 \ ; \tag{3-7a}$$

for this particular case (3-3) gives

$$\chi = \kappa \ , \tag{3-7b}$$

which justifies the name, curvature parameter, for χ (in the general case $C_o \neq 1$, $\xi \neq 1$, χ is not the curvature itself but related to it by (3-3)).

As we shall see (Table 3-3), the three parameters C_o, ξ, and χ characterize very well the behavior of a covariance function for small and medium distances. Two different functions having the same numerical values for C_o, ξ and χ, will give very nearly the same interpolation errors. In fact, the variance C_o determines, so to speak, the scale of interpolation errors; the curvature parameter χ characterizes the behavior for small distances s, and the correlation length ξ describes the behavior at medium distances s on the order of ξ itself.

Thus the description of $C(s)$ by C_o and ξ only is not satisfactory since the curvature at the origin influences essentially the interpolation for small distances s.

The curvature parameter χ is also essential with the use of gradients. As we have seen in the preceding section, the function

$$-C''(s) = 2a_1 - 12a_2s^2 + - \ldots \tag{3-8}$$

denotes the covariance function for the horizontal gradient, that is, for $\partial\Delta g/\partial y$ if $C(s)$ is the covariance function of the gravity anomaly. Thus the variance of $\partial\Delta g/\partial y$, denoted by G_o, is given by

$$G_o = 2a_1 \ . \tag{3-9}$$

This equation, together with (3-6), gives

$$\chi = G_o \xi^2 / C_o \; . \tag{3-10}$$

This basic relation expresses the curvature parameter in terms of the variances C_o, of Δg , and G_o , of $\partial\Delta g/\partial x$, together with the correlation length of $C(s)$.

As an example, assume

$$\begin{aligned} C_o &= 1500 \text{ mgal}^2 , \\ G_o &= 200 \text{ E}^2 , \\ \xi &= 50 \text{ km} . \end{aligned} \tag{3-11}$$

Since, for Eötvos units E ,

$$1 \text{ E} = 0.1 \text{ mgal/km} , \tag{3-12}$$

the expression (3-10) gives

$$\chi = \frac{10}{3} = 3.33333 \; . \tag{3-13}$$

Thus the relation (3-10) is of fundamental importance for an empirical determination of χ . It also shows that a bad choice of covariance functions with respect to χ completely falsifies the gradient variance.

Let us now compute ξ and χ for the simple covariance models considered in the preceding section. Hirvonen's covariance function (2-21),

$$C(s) = \frac{C_o}{1+(s/d)^2} \tag{3-14}$$

has the correlation length

$$\xi = d \tag{3-15}$$

and the series expansion

$$C(s) = C_o - \frac{C_o}{d^2}s^2 \ldots \tag{3-16}$$

Thus (3-6) gives

$$\chi = 2 \ . \tag{3-17}$$

For the Gaussian function (2-26),

$$C(s) = C_o e^{-A^2 s^2} \ , \tag{3-18}$$

we have

$$\xi = \frac{1}{A}\sqrt{\ln 2} \ . \tag{3-19}$$

From the series expansion

$$C(s) = C_o - C_o A^2 s^2 \ldots \tag{3-20}$$

we get

$$a_1 = C_o A^2$$

and hence, from (3-6) and (3-19)

$$\chi = 2A^2 \xi^2 = 2\ln 2 = 1.38629 \ . \tag{3-21}$$

The cosine function (2-35),

$$C(s) = C_o \cos\beta s \ , \tag{3-22}$$

has $\beta\xi = 60^\circ = \frac{\pi}{3}$, whence

$$\xi = \frac{\pi}{3\beta} = 1.04720\beta^{-1} . \tag{3-23}$$

From

$$C(s) = C_o - \frac{1}{2}C_o\beta^2 s^2 \ldots \tag{3-24}$$

we derive

$$\chi = \frac{\pi^2}{9} = 1.09662 . \tag{3-25}$$

Let us now consider a generalization of Hirvonen's model (3-14), namely the function

$$C(s) = \frac{C_o}{(1+A^2s^2)^m} , \tag{3-26}$$

where the parameter m is allowed to assume positive real values. The correlation length ξ is given by

$$\xi = \frac{1}{A}(2^{\frac{1}{m}}-1)^{\frac{1}{2}} , \tag{3-27}$$

and from the series expansion

$$C(s) = C_o - mC_oA^2s^2 \ldots \tag{3-28}$$

we get

$$\chi = 2m(2^{\frac{1}{m}}-1) . \tag{3-29}$$

The following Table 3-1 shows some values of χ for different n :

Table 3-1

m	χ
0.1	204.6
0.2	12.4
0.5	3
1	2

m	χ
1.5	1.76220
2	1.65685
10	1.43547
∞	1.38629

For $m \to \infty$, the function (3-26) tends to the exponential function (3-18) (provided the scale of s is suitably chosen), and (3-29) becomes

$$\chi = \lim_{m\to\infty} 2m(2^{\frac{1}{m}}-1) = 2\ln 2 = 1.38629 \ , \qquad (3\text{-}30)$$

which is the value (3-21).

The function (3-26) satisfies the condition (2-30) for positive definiteness for an arbitrary parameter $m > 0$. It is able to model an empirical covariance function for arbitrary $\chi > 1.38629$; however, the use of (3-26) for general m is restricted to covariance functions defined in the plane only, since spatial extensions are known only for the values $m = 1/2$ and $m = 3/2$; see the following section.

Finally we consider a covariance model of a different kind, which will be discussed further in sec. 4:

$$C(s) = \frac{C_o}{A} \ln \frac{2e^A}{1 + \sqrt{1+k^2 s^2}} \quad , \tag{3-31}$$

with parameters C_o (variance), A and k. The correlation length ξ is determined by

$$\xi = k^{-1}\left[(2e^{A/2}-1)^2 - 1\right]^{\frac{1}{2}} \quad , \tag{3-32}$$

and the series expansion of (3-31) starts with

$$C(s) = C_o - \frac{C_o}{4A}k^2 s^2 \; \ldots \quad , \tag{3-33}$$

whence

$$\chi = \frac{1}{2A}k^2\xi^2 = \frac{1}{2A}\left[(2e^{A/2}-1)^2 - 1\right] \; . \tag{3-34}$$

The following Table 3-2 shows some values of χ for different parameters A.

Table 3-2

A	χ
0.001	1.0008
0.1	1.0780
1	2.1391
5	54.4923

This function is able to model an empirical covariance function for any curvature parameter χ greater than

$$x_o = \lim_{A \to o} \frac{1}{2A}\left[(2e^{A/2}-1)^2 - 1\right] = 1 . \qquad (3\text{-}35)$$

As we shall see in the following section, this covariance function can very simply be extended into space. Its series expansion satisfies the condition (2-20) for positive definiteness, but condition (2-36) is violated for $s \geqq s_o$ where

$$s_o = k^{-1}\left[(2e^{2A}-1\ \ ^2)- 1\right]^{\frac{1}{2}}; \qquad (3\text{-}36)$$

therefore, the model (3-31) cannot be used for distances much larger than the correlation length ξ .

So far we have considered very different analytical models for covariance functions. To see whether the three "essential" parameters C_o (variance), ξ (correlation distance) and χ (curvature parameter) really characterize the behavior of a covariance function, let us compare two very different functions, the Gaussian function (3-18) and the logarithmic model (3-31). They are normalized such as to have

$$C_o = 1 , \qquad \xi = 1 .$$

These values and χ given by (3-21) are in common to both functions. Table 3-3 gives a table of values for both functions $C_1(s)$, which is the Gaussian function (3-18), and $C_2(s)$, which is the logarithmic function (3-31).

Table 3-3

s	$C_1(s)$	$C_2(s)$
0.0	1.0000	1.0000
0.1	0.9931	0.9931
0.2	0.9727	0.9728
0.3	0.9395	0.9400
0.4	0.8950	0.8963
0.5	0.8409	0.8435
0.6	0.7792	0.7833
0.7	0.7120	0.7175
0.8	0.6417	0.6475
0.9	0.5704	0.5747
1.0	0.5000	0.5000
1.1	0.4323	0.4244
1.2	0.3686	0.3484
1.3	0.3099	0.2726
1.4	0.2570	0.1973
1.5	0.2102	0.1229
1.6	0.1696	0.0495
1.7	0.1349	-0.0227
1.8	0.1058	-0.0937
1.9	0.0819	-0.1633
2.0	0.0625	-0.2315

The agreement for $s \leqq \xi = 1$ is excellent indeed. Comparisons between other functions of the same C_o, ξ, and χ give similarly good results.

Conclusions.- We have seen that the three parameters C_o, ξ, and χ are necessary and sufficient for a practically satisfactory characterization of a covariance function for local applications, that is, for distances not much larger than the correlation length ξ .

The chosen analytical covariance model must, therefore, be fitted to the empirical values of these parameters. With respect to C_o and ξ , such a fit is not difficult since it corresponds only to a change of scales. More difficult, but no less essential, is a good fit with respect to χ .
It may happen that we do not have a suitable model for the desired χ , but two different possible models $C_1(s)$ and $C_2(s)$ with the two curvature parameters χ_1 and χ_2 , respectively, such that $\chi_1 \leqq \chi \leqq \chi_2$. Then a solution is found as follows. Put first $C_o = 1$ and $\xi = 1$ for both models. Express the given χ as a linear combination of χ_1 and χ_2 :

$$\chi = \lambda\chi_1 + (1-\lambda)\chi_2 \tag{3-37}$$

where

$$0 \leqq \lambda = \frac{\chi_2 - \chi}{\chi_2 - \chi_1} \leqq 1 \; . \tag{3-38}$$

Then the function

$$C(s) = \lambda C_1(s) + (1-\lambda)C_2(s) \tag{3-39}$$

will have the desired curvature parameter χ and again $C_o = 1$ and $\xi = 1$. This follows at once by expanding both covariance functions $C_1(s)$ and $C_2(s)$ into power series, the first two terms being sufficient, and substituting them into (3-39). (That a linear combination (3-39) of two covariance functions with positive coefficients λ and $1-\lambda$ is again a covariance function, that is, a positive definite function, is immediately seen from the spectra: if the spectra of $C_1(s)$ and $C_2(s)$ are nonnegative, then the spectrum of $C(s)$, being a linear combination of these two spectra with positive coefficients, will also be nonnegative.)

The curvature parameter χ represents the curvature at the origin $s = 0$ of the covariance curve for fixed $C_o = 1$ and $\xi = 1$. A small value of χ corresponds to a well-rounded, rather flat mountain top, a large value of χ to a pronounced peak. Whereas no theoretical upper limit for χ exists (the peak may be arbitrarily sharp), it is intuitively obvious that the mountain top may not be arbitrarily flat. The lower limit for χ seems to be on the order of 1; cf. (3-25) and (3-35).

An empirical determination of χ is possible by (3-10), using the gradient variance.

As a matter of fact, the three parameters C_o, ξ, and χ characterize only the local behavior of a covariance function for, say, the gravity anomaly Δg. If other covariance functions are derived from such a covariance function by covariance propagation, then additional parameters may become important, and more sophisticated spatial covariance models must be constructed. However, even in these more general circumstances, the three parameters C_o, ξ, and χ will retain a basic role.

4. Spatial Covariance Models

In the present section we shall consider some simple rotationally symmetric spatial harmonic covariance functions and their planar equivalents.

By putting

$$k_n = \kappa_n \left(\frac{R_B}{R}\right)^{2n+1} \tag{4-1}$$

we may transform the basic expression (1-1) into the form

$$K(P,Q) = \sum_{n=o}^{\infty} \kappa_n \left(\frac{R_B^2}{r_P r_Q}\right)^{n+1} P_n(\cos\psi) \ . \tag{4-2}$$

Here $R_B < R$ is the radius of some sphere completely inside the terrestrial sphere of radius R ; the sphere of radius R_B is frequently called "Bjerhammar sphere".

By means of the substitution

$$\sigma = \frac{R_B^2}{r_P r_Q} \ , \tag{4-3}$$

the covariance function may simply be written as

$$K(P,Q) = \sum_{n=o}^{\infty} \kappa_n \sigma^{n+1} P_n(\cos\psi) \ . \tag{4-4}$$

We shall now consider some cases in which this series can be summed in closed form, namely the cases $\kappa_n = 1$, $\kappa_n = 2n+1$ and $\kappa_n = 1/n$.

The Reciprocal Distance Covariance Function. - If

$$\kappa_n = 1 \tag{4-5}$$

for all n, then

$$K(P,Q) = \sum_{n=0}^{\infty} \sigma^{n+1} P_n(\cos\psi) \tag{4-6}$$

may be summed by means of the well-known expression for the reciprocal distance, cf. (Heiskanen and Moritz, 1967, p.33). Equation (1-81) in that book gives immediately

$$K(P,Q) = \sigma(1 - 2\sigma\cos\psi + \sigma^2)^{-\frac{1}{2}} . \tag{4-7}$$

Therefore, this function will be called "reciprocal distance covariance function", although it is not simply the reciprocal spatial distance between points P and Q.

In a certain sense, the function (4-7) is the simplest possible rotationally symmetric harmonic covariance function; it is defined outside the Bjerhammar sphere $r = R_B$, that is, for $\sigma < 1$. It has already been considered by Krarup (1969, p.62).

For applications in limited areas~~s,~~ it is possible and sometimes useful to replace the sphere $r = R$ by its tangential plane.

To perform a suitable transition from the sphere to the plane, we put

$$\zeta = 1 - \sigma , \tag{4-8}$$

$$\lambda = 2\sin\frac{\psi}{2} , \tag{4-9}$$

and

$$L = (1 - 2\sigma\cos\psi + \sigma^2)^{\frac{1}{2}} . \tag{4-10}$$

Since

$$\cos\psi = 1 - 2\sin^2\frac{\psi}{2} = 1 - \frac{1}{2}\lambda^2 , \tag{4-11}$$

we have

$$L^2 = (1 - \sigma)^2 + \sigma\lambda^2$$

or

$$L^2 = \zeta^2 + \sigma\lambda^2. \tag{4-12}$$

This expression is still rigorous. We now put

$$\begin{aligned} r_P &= R + z_P , \\ r_Q &= R + z_Q , \\ R_B &= R - b/2 . \end{aligned} \tag{4-13}$$

Then (4-3) gives

$$\sigma = \frac{(R-b/2)^2}{(R+z_P)(R+z_Q)} = 1 - \frac{z_P+z_Q+b}{R} + \ldots \tag{4-14}$$

Neglecting second-order terms we thus get from (4-8)

$$\zeta = \frac{z_P+z_Q+b}{R} . \tag{4-15}$$

To a similar approximation, (4-9) gives

$$\lambda = \frac{s}{R} , \tag{4-16}$$

where s denotes horizontal distance as usual. Thus (4-10) becomes

$$\frac{1}{L} = \frac{R}{\sqrt{s^2 + (z_P + z_Q + b)^2}} \left[1 + O(\zeta) \right] \quad , \tag{4-17}$$

where $O(\zeta)$ denotes terms of order ζ or smaller. Disregarding a relative error of $O(\zeta)$ and admitting a constant factor B/R we thus find the <u>planar equivalent</u> of (4-7):

$$K(P,Q) = \frac{B}{D} \quad , \tag{4-18}$$

where

$$D^2 = (x_B - x_A)^2 + (y_B - y_A)^2 + (z_A + z_B + b)^2 \quad . \tag{4-19}$$

This function has been used and discussed at length in (Moritz, 1974, sec.3). By means of the substitutions

$$\begin{aligned} X &= x_B - x_A \ , \\ Y &= y_B - y_A \ , \\ Z &= z_A + z_B + b \end{aligned} \tag{4-20}$$

we have

$$s^2 = X^2 + Y^2 \tag{4-21}$$

and

$$D^2 = Y^2 + Y^2 + Z^2 \quad . \tag{4-22}$$

For $z_A = z_B =$ const. we have $Z =$ const., so that (4-18) becomes

$$K(s) = \frac{B/Z}{(1 + s^2/Z^2)^{1/2}} \quad , \tag{4-23}$$

which is of the form (3-26), with

$$C_o = \frac{B}{Z} \quad , \quad A = \frac{1}{Z} \quad , \quad m = \frac{1}{2} \quad . \tag{4-24}$$

For different elevations $z_A = z_B$, the covariance function has the same form (4-23), but with parameters varying with elevation. For increasing elevation, the variance decreases and the curve flattens out: the correlation length ξ , given by

$$\xi = Z\sqrt{3} \tag{4-25}$$

according to (3-27), is proportional to Z . On the other hand, the curvature parameter is always

$$\chi = 3 \quad , \tag{4-26}$$

independently of elevation. Therefore, this function can be directly used only if the empirical value of happens to be around 3.

The advantage of the function (4-18) is that it can be easily handled analytically. It can be differentiated in a simple way, as shown in (Moritz, 1974, sec.3); in this manner it is readily verified that the function is harmonic. By repeated differentiation with respect to z_A and z_B we may derive new covariance functions (for first and second vertical gradients):

$$C_z(P,Q) = K_o\left(-\frac{1}{D^3} + \frac{3}{D^5}Z^2\right) , \tag{4-27}$$

$$C_{zz}(P,Q) = K_o\left(\frac{9}{D^5} - \frac{90}{D^7}Z^2 + \frac{105}{D^9}Z^4\right) \tag{4-28}$$

(*ibid*., sec.4).

By means of the series expansions given *ibid*., p.25 and the correlation distances given in Table 4-1 (*ibid*., p.24) we find for $C_z(P,Q)$:

$$\chi = 1.5 , \tag{4-29}$$

and for $C_{zz}(P,Q)$:

$$\chi = 1.35 . \tag{4-30}$$

By successive differentiations it is thus possible to obtain covariance functions with decreasing χ .

This gives a limited flexibility for fitting spatial covariance functions to empirical covariance functions, provided the given χ has one of the values 3, 1.5, 1.35, ... For instance, we may use (4-18) for T , (4-27) for $T_z \doteq \Delta g$, and (4-28) for T_{zz} ; or also (4-18) for T_z , (4-27) for T_{zz} , and (4-28) for T_{zzz} ; etc. However, nothing can be done with this model for $\chi > 3$.

Since for small s , the spherical and planar covariance functions agree, the χ-values given hold also for the corresponding spherical functions.

The Poisson Covariance Function.- We now take

$$\kappa_n = 2n+1 .$$

Then (4-4) becomes

$$K(P,Q) = \sum_{n=0}^{\infty} (2n+1)\sigma^{n+1} P_n(\cos\psi) \quad . \tag{4-31}$$

By differentiating the identity (cf.(4-6),(4-7),(4-10))

$$\frac{2}{L} = 2\sum_{n=0}^{\infty} \sigma^n P_n(\cos\psi)$$

with respect to σ, multiplying by σ^2 and adding σ/L we get

$$\sigma^2 \frac{\partial}{\partial\sigma}\left(\frac{2}{L}\right) + \frac{\sigma}{L} = \sum_{n=0}^{\infty} (2n+1)\sigma^{n+1} P_n(\cos\psi) \quad .$$

The left-hand side can be computed, so that (4-31) becomes

$$K(P,Q) = \frac{\sigma(1-\sigma^2)}{L^3} \quad . \tag{4-32}$$

This is the desired closed expression for the sum of (4-31).

The function (4-32) may be called <u>Poisson covariance function</u>, because essentially it represents the kernel in the well-known Poisson integral (cf. Heiskanen and Moritz, 1967, p.35). It has also been given already in (Krarup, 1969, p.43).

The planar approximation is again readily found. By (4-8) we have

$$1-\sigma^2 = (1+\sigma)(1-\sigma) \doteq 2\zeta + O(\zeta^2) \quad . \tag{4-33}$$

Using (4-14), (4-15), (4-17), (4-20) and (4-33) we get

$$\frac{\sigma(1-\sigma^2)}{L^3} = \frac{2ZR^2}{(s^2+Z^2)^{3/2}}\left[1 + O(\zeta)\right] \quad .$$

Neglecting a relative error of $\zeta = Z/R$ and admitting a constant factor we thus have

$$K(P,Q) = \frac{BZ}{(s^2+Z^2)^{3/2}} \tag{4-34}$$

as the planar equivalent of (4-32). Here B is a constant, and Z is given by (4-20).

Writing (4-34) for $Z = \text{const.}$ as

$$K(s) = \frac{B/Z^2}{(1 + s^2/Z^2)^{3/2}} \quad , \tag{4-35}$$

we recognize the form (3-26) with $m = 3/2$. The curvature parameter is, therefore, given by (3-29):

$$\chi = 1.76220 \; . \tag{4-36}$$

Again we could derive new spatial harmonic covariance models by differentiation, but these derived models do not seem to present any novel features.

More interesting is the question whether the functions (4-23), with $m = 1/2$, and (4-35), with $m = 3/2$, are the only plane covariance functions of form (3-26) which possess a natural extension into space. In other terms, are there harmonic spatial covariance functions of the form

$$K(P,Q) = \frac{BZ^\alpha}{(s^2+Z^2)^\beta} \quad , \tag{4-37}$$

other than (4-18) and (4-34)? To find this out, we must form the Laplacian of (4-37),

$$\Delta_P K = \frac{\partial^2 K}{\partial x_P^2} + \frac{\partial^2 K}{\partial y_P^2} + \frac{\partial^2 K}{\partial z_P^2} \quad , \tag{4-38}$$

and similarly $\Delta_Q K$. From (4-20) we see that

$$\Delta_P K = \Delta_Q K = \frac{\partial^2 K}{\partial X^2} + \frac{\partial^2 K}{\partial Y^2} + \frac{\partial^2 K}{\partial Z^2} = \Delta K \ . \tag{4-39}$$

On performing the appropriate differentiations of (4-37) we find

$$\Delta K = 2\beta(-2\alpha+2\beta-1)\frac{Z^\alpha}{(Z^2+s^2)^{\beta+1}} + \alpha(\alpha-1)\frac{Z^{\alpha-2}}{(Z^2+s^2)^\beta} \ . \tag{4-40}$$

This expression will be identically zero for arbitrary Z and s if and only if the coefficients are zero, that is, for

$$\begin{aligned} &\alpha(\alpha-1) = 0 \ , \\ &2\beta(-2\alpha+2\beta-1) = 0 \ . \end{aligned} \tag{4-41}$$

The only nontrivial solutions of these two equations are

$$\alpha = 0 \ , \qquad \beta = 1/2 \tag{4-42}$$

and

$$\alpha = 1 \ , \qquad \beta = 3/2 \ , \tag{4-43}$$

the first corresponding to (4-18) and the second to (4-34); there are no other solutions.

This does not mean that spatial extensions of other plane functions of form (3-26) do not exist; they only do not have the simple form (4-37) and it does not seem worthwile to study them in this context.

The Logarithmic Covariance Function.- Finally we take

$$\kappa_n = \frac{1}{n} \qquad (n \geqq 1) \ . \tag{4-44}$$

Then (4-4) becomes

$$K(P,Q) = \sum_{n=1}^{\infty} \frac{1}{n} \sigma^{n+1} P_n(\cos\psi) \ . \tag{4-45}$$

For this function we have

$$\frac{\partial}{\partial\sigma}\left(\frac{K(P,Q)}{\sigma}\right) = \sum_{n=1}^{\infty} \sigma^{n-1} P_n(\cos\psi) \ ,$$

so that

$$\sigma\frac{\partial}{\partial\sigma}\left(\frac{K}{\sigma}\right) + 1 = \sum_{n=0}^{\infty} \sigma^{n} P_n(\cos\psi) = \frac{1}{L} \tag{4-46}$$

or

$$\frac{\partial}{\partial\sigma}\left(\frac{K}{\sigma}\right) = \frac{1}{\sigma}\left(\frac{1}{L} - 1\right) \ . \tag{4-47}$$

The function

$$K(P,Q) = \sigma \ln \frac{2}{N} \ , \tag{4-48}$$

where

$$N = 1 + L - \sigma \cos\psi \ , \tag{4-49}$$

is readily seen to satisfy (4-47) and the boundary condition

$$K(P,Q) = 0 \quad \text{for} \quad \sigma = 0 \ . \tag{4-50}$$

It represents, therefore, the desired sum of (4-45).

Covariance functions of this and similar types have been employed by Tscherning (1972) and Lauritzen (1973).

Let us now study the logarithmic covariance function (4-48) in some detail. By (4-8), (4-9), (4-12) and (4-49) we have rigorously

$$N = \zeta + \frac{1}{2}\sigma\lambda^2 + \sqrt{\sigma\lambda^2 + \zeta^2} \ , \tag{4-51}$$

where

$$\lambda = 2\sin\frac{\psi}{2} \ , \tag{4-52}$$

$$\zeta = 1 - \sigma \ , \tag{4-53}$$

$$\sigma = \left(\frac{R_B}{R}\right)^2 , \tag{4-54}$$

assuming $r_P = r_Q = R$ in (4-3).

For $\psi = 0$ we have $\lambda = 0$ and therefore, by (4-51),

$$N_o = 2\zeta \ , \tag{4-55}$$

so that (4-48) gives the variance

$$K_o = \sigma \ln \frac{1}{\zeta} \ . \tag{4-56}$$

For $\psi = \pi$ we have $\lambda = 2$ and hence by (4-51)

$$N_\pi = 2 - \zeta + \sqrt{4 - 4\zeta + \zeta^2} \ , \tag{4-57}$$

taking (4-53) into account. For $\psi = \pi$, (4-48) gives

$$K_\pi = \sigma \ln \frac{2}{N_\pi} \ . \tag{4-58}$$

Hence,

$$\frac{K_\pi}{K_o} = \frac{\ln(2/N_\pi)}{\ln(1/\zeta)} = \frac{\ln(N_\pi/2)}{\ln \zeta} \ . \tag{4-59}$$

On expanding (4-57) into a power series for small ζ we get

$$N_\pi = 4 - 2\zeta \ \ldots \ ,$$

$$\ln(N_\pi/2) = \ln 2 + O(\zeta) \ ,$$

so that (4-59) becomes approximately

$$\frac{K_\pi}{K_o} = \frac{\ln 2}{\ln \zeta} \ , \tag{4-60}$$

which is small for small ζ. Thus, the function $K(P,Q)$ is well-behaved even for $\psi = \pi$, that is for maximum distances along the sphere $r = R$.

Let us now determine the correlation length ξ, that is, the value of λ for which

$$K(\xi) = \tfrac{1}{2}K_o \, . \qquad \text{(4-6}$$

The condition is

$$\ln\frac{2}{N_\xi} = \frac{1}{2}\ln\frac{1}{\zeta}$$

or

$$N_\xi = 2\sqrt{\zeta} \, . \qquad \text{(4-6}$$

Using (4-51) this becomes

$$\zeta + \frac{1}{2}\sigma\xi^2 + \sqrt{\sigma\xi^2+\zeta^2} = 2\sqrt{\zeta} \qquad \text{(4-6}$$

or

$$\sqrt{w + \zeta^2} = \mu - \frac{1}{2}w \, , \qquad \text{(4-6}$$

where we have put

$$\mu = 2\sqrt{\zeta} - \zeta \, , \qquad \text{(4-6}$$

$$w = \sigma\xi^2 \, . \qquad \text{(4-6}$$

From (4-64) we get a quadratic equation for w :

$$w^2 - 4(1+\mu)w + 4(\mu^2-\zeta^2) = 0 \qquad \text{(4-6}$$

with solution

$$w = 2(1+\mu \pm \sqrt{1+2\mu+\zeta^2}) . \tag{4-68}$$

Since the plus root would correspond to $\psi > \pi$, which is impossible, we retain the minus root and expand again in a series with respect to μ and ζ , obtaining

$$w = 4\zeta(1 - \sqrt{\zeta}) + O(\zeta^2) . \tag{4-69}$$

Thus, the correlation distance ξ is obtained from

$$\sigma\xi^2 = 4\zeta(1 - \sqrt{\zeta}) + O(\zeta^2) . \tag{4-70}$$

Let us now determine the curvature parameter χ . We expand (4-51) for small λ , obtaining

$$N = 2\zeta\left[1 + \frac{1+\zeta}{4\zeta^2}\sigma\lambda^2 \ldots\right] , \tag{4-71}$$

whence

$$\begin{aligned} \ln\frac{N}{2} &= \ln\zeta + \frac{1+\zeta}{4\zeta^2}\sigma\lambda^2 \ldots \\ &= \ln\zeta\left[1 - \frac{1+\zeta}{4\zeta^2\ln\zeta^{-1}}\sigma\lambda^2 \ldots\right] . \end{aligned} \tag{4-72}$$

In view of (4-48) and (3 -6), this gives rigorously

$$\chi = \frac{1+\zeta}{2\zeta^2\ln\zeta^{-1}}\sigma\xi^2 , \tag{4-73}$$

and by (4-70) we get for small ζ , approximately,

$$\chi = \frac{2}{\zeta \ln \zeta^{-1}} \quad .$$

Let us illustrate these formulas by means of an example. Assume a correlation length of 63.7 km; in radians this corresponds to

$$\xi = \frac{63.7\,\text{km}}{6370\,\text{km}} = 0.01 \quad .$$

For this we must select ζ according to (4-70) such that

$$\zeta \doteq \frac{1}{4}\xi^2 = 0.000\,025 \quad ,$$

which corresponds to

$$R_B = 0.999\,9875\ R \quad .$$

Then (4-74) gives

$$\chi = 7550 \quad ,$$

which is obviously an unrealistically high value. However, we might linearly combine a function of type (4-7), with $\chi = 3$, and a function of type (4-48), with $\chi = 7550$, to obtain a covariance function with any desired intermediate χ , as explained at the end of sec.3.

Finally we shall derive the corresponding planar covariance function, proceeding as we did before. The rigorous expression (4-51) is transformed by substituting, as usual,

$$\lambda = \frac{s}{R} ,$$

$$\zeta = \frac{Z}{R} ,$$

with the result

$$N = \frac{1}{R}\left[Z + \frac{s^2}{2R}(1-\frac{Z}{R}) + \sqrt{s^2(1-\frac{Z}{R}) + Z^2}\right]$$

$$= \frac{1}{R}(Z + \sqrt{s^2 + Z^2})\left[1 + 0(\frac{Z}{R})\right] .$$

Substituting into (4-48), disregarding an error of $0(Z/R)$ and admitting a constant factor B we obtain

$$K(P,Q) = B\ln\frac{2R}{Z + \sqrt{s^2+Z^2}} . \tag{4-79}$$

This function is a spatial covariance function. By straightforward differentiation it is not difficult to verify that it satisfies Laplace's equation. By differentiating it twice with respect to Z, we get the covariance function for the first-order vertical gradient, which will be seen to be identical to (4-34), apart from a constant factor.

Let us finally write (4-79) in the form

$$K(PQ) = B\ln\frac{2R/Z}{1 + \sqrt{1+s^2/Z^2}} \tag{4-80}$$

and introduce new constants by

$$C_o = B\ln(R/Z) ,$$

$$A = \ln(R/Z) \ , \qquad (4\text{-}8$$

$$k = \frac{1}{Z} \ ,$$

assuming $Z = \text{const}$. Then (4-80) becomes

$$K(s) = \frac{C_o}{A} \ln \frac{2e^A}{1 + \sqrt{1+k^2 s^2}} \ , \qquad (4\text{-}8$$

which is the form (3-31) used in the preceding section.

Simple generalizations of (4-45) are the functions

$$F_i = \sum_{n_o}^{\infty} \frac{\sigma^{n+1}}{n+i} P_n(\cos\psi) \ , \qquad (4\text{-}8$$

where i denotes any integer and

$$n_o = 0 \qquad \text{for} \quad i > 0 \ ,$$

$$n_o = -i+1 \qquad \text{for} \quad i < 0 \ . \qquad (4\text{-}8$$

These functions have been studied in (Tscherning and Rapp, 1974, pp.31-38). It is not difficult to show that all these functions lead to the same plane equivalent (4-79). Thus they have the same local behavior as (4-45), although they differ on a global scale.

Functions such as (4-6), (4-31) and (4-83) may be considered as building blocks, from which we can construct covariance functions that have given properties, such as prescribed degree variances (Tscherning and Rapp, 1974).

The purpose of the present study has been mainly to investigate the local behavior of different covariance function models. By prescribing the local behavior in terms of the basic parameters C_o, ξ and χ as defined in sec. 3, and the global behavior in terms of degree variances, geoid height variance and other quantities, it should be possible to construct, from the building blocks mentioned, suitable covariance functions that can be used for local as well as for global applications.

PART B

ON THE INFLUENCE OF COVARIANCES ON THE RESULTS OF COLLOCATION

5. Accuracy of Collocation Using a "Wrong" Covariance Function

What happens if an incorrect covariance function is used in least-squares collocation? The answer to this question is obviously of great practical importance, since the "true" covariance function is never exactly known, so that it must always be replaced by an analytical approximation.

Let us introduce the following notation, which will be consistently used throughout Part B of the present report:

K ... true covariances,
C ... computational covariances.

The "computational covariance function" $C(P,Q)$ is an analytical expression approximating the unknown true covariance function $K(P,Q)$; the function $C(P,Q)$ is the covariance function used in computing the least-squares collocation estimates:

$$s_P = \underline{C}_P^T \underline{C}^{-1} \underline{x} \ . \tag{5-1}$$

This is formula (2-38) of (Moritz, 1972, p.15); systematic parameters $\underline{X}$ are supposed to be absent.

Equation (5-1) is explicitly written as

$$s_P = \left[C_{P1} C_{P2} \; \dots \; C_{Pn} \right] \begin{bmatrix} \bar{C}_{11} \bar{C}_{12} & \dots & \bar{C}_{1n} \\ \bar{C}_{21} \bar{C}_{22} & \dots & \bar{C}_{2n} \\ \vdots & & \vdots \\ \bar{C}_{n1} \bar{C}_{n2} & \dots & \bar{C}_{nn} \end{bmatrix}^{-1} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} . \qquad (5\text{-}2)$$

Here s_P is the signal to be estimated and the x_i are the measurements; both s_P and x_i may be any quantities of the anomalous gravity field such as geoidal heights, deflections of the vertical, gravity anomalies, higher-order anomalous gradients, etc. The C_{Pi} and $\bar{C}_{ik}$ are computational covariances:

$$C_{Pi} = \mathrm{cov}(s_P, x_i) \; , \qquad (5\text{-}3)$$

$$\bar{C}_{ik} = \mathrm{cov}(x_i, x_k) = C_{ik} + D_{ik} \; . \qquad (5\text{-}4)$$

The C_{Pi} and C_{ik} are signal covariance obtained from the computational covariance function $C(P,Q)$; the D_{ik} are covariances of measuring errors. The row vector $\underline{C}_P^T$ is the transpose of the column vector $\underline{C}_P$ formed by the covariances C_{Pi} .

We shall now proceed similarly as in (Moritz, 1972, p.28). The expression (5-1) may be abbreviated as

$$s_P = \underline{Lx} \qquad (5\text{-}5)$$

where

$$\underline{L} = \underline{C}_P^T \underline{\bar{C}}^{-1} \; . \qquad (5\text{-}6)$$

Then the individual error of the estimated signal s_P is given by

$$\varepsilon_P = \bar{s}_P - s_P = \bar{s}_P - \underline{L}\underline{x} , \tag{5-7}$$

where $\bar{s}_P$ represents the true value of the signal s_P .

The square of (5-7) is

$$\varepsilon_P^2 = \bar{s}_P^2 - 2\underline{L}\bar{s}_P\underline{x} + \underline{L}\underline{x}\underline{x}^T\underline{L}^T . \tag{5-8}$$

We now form the mean values M :

$$M\{\varepsilon_P^2\} = m_P^2 , \tag{5-9}$$

$$M\{\bar{s}_P^2\} = K_o , \tag{5-10}$$

$$M\{\bar{s}_P\underline{x}\} = \underline{K}_P , \tag{5-11}$$

$$M\{\underline{x}\underline{x}^T\} = \underline{\bar{K}} . \tag{5-12}$$

Here m_P^2 denotes the mean square error of estimation, K_o denotes the variance of the signal s_P , and the matrices $\underline{K}_P$ and $\underline{\bar{K}}$ correspond to $\underline{C}_P$ and $\underline{\bar{C}}$ as defined by (5-3) and (5-4), but they are now the true covariances.

Therefore the mean of (5-8) gives

$$m_P^2 = K_o - 2\underline{L}\underline{K}_P + \underline{L}\underline{\bar{K}}\underline{L}^T . \tag{5-13}$$

On substituting (5-6) this becomes finally

$$m_P^2 = K_o - 2\underline{C}_P^T\underline{\bar{C}}^{-1}\underline{K}_P + \underline{C}_P^T\underline{\bar{C}}^{-1}\underline{\bar{K}}\underline{\bar{C}}^{-1}\underline{C}_P . \tag{5-14}$$

This formula expresses the standard error of estimation in terms of the true covariances K and the computational covariances C actually used in the computations.

It seems appropriate to keep in mind the precise meaning of the estimation formula (5-1). If the computational covariances differ from the true covariances K, then the formal solution (5-1) no longer represents the <u>optimal</u> least-squares collocation estimate in the strict sense, which would be

$$\hat{s}_P = \underline{K}_P^T \underline{\bar{K}}^{-1} \underline{x} \ . \tag{5-15}$$

The "wide-sense collocation" formula (5-1) is to be considered as a formal solution which interpolates the given data and possesses all advantages of the optimal solution (5-15), such as consistency of the mathematical model, harmonicity, etc., with the <u>only</u> exception of optimal accuracy, which is reserved to the "strict-sense collocation" formula (5-15).

The standard error $\hat{m}_P$ corresponding to (5-15) is obtained by putting $C = K$ in (5-14):

$$\hat{m}_P^2 = K_o - \underline{K}_P^T \underline{\bar{K}}^{-1} \underline{K}_P \ . \tag{5-16}$$

This is a well-known formula; cf. (Moritz, 1972, p.33), putting $\underline{A} = 0$ in eq.(3-36).

It is sometimes useful to have an explicit expression for the difference m_P^2 (actual) minus $\hat{m}_P^2$ (optimal). From (5-14) and (5-16) we get by suitable rearrangement

$$m_P^2 - \hat{m}_P^2 = (\underline{K}_P^T \underline{\bar{K}}^{-1} - \underline{C}_P^T \underline{\bar{C}}^{-1}) \underline{\bar{K}} (\underline{\bar{K}}^{-1} \underline{K}_P - \underline{\bar{C}}^{-1} \underline{C}_P) . \tag{5-17}$$

This formula, which can be immediately verified, is nothing but a special case of eq.(3-52b) of (Moritz, 1972, p.37). It shows that always

$$\bar{m}_P \leqq m_P \tag{5-18}$$

since the right-hand side of (5-17) is always positive in view of the positive definiteness of $\underline{K}$.

We finally note that, if C and K differ considerably, it would be wrong to calculate m_P^2 by the expression

$$C_o - \underline{C}_P^T \underline{C}^{-1} \underline{C}_P \tag{5-19}$$

analogous to (5-16): even if the C are used in computation, a meaningful accuracy estimate must involve the true covariances K , so that (5-14) has to be used.

6. Application of Stepwise Collocation

It is frequently convenient to split up the estimation by collocation into two steps, just as in ordinary least-squares adjustment. This may be done to reduce the size of matrices to be inverted; another application is the use of additional observations to improve the original estimates.

Stepwise collocation has been treated in (Moritz, 1973) with respect to the estimate (5-1) and the simple standard error formula (5-16). We shall now apply stepwise collocation to the new expression (5-14) for the standard error of collocation using a "wrong" covariance function.

This formula is

$$m_P^2 = K_o - 2\underline{C}_P^T \underline{\bar{C}}^{-1} \underline{K}_P + \underline{C}_P^T \underline{\bar{C}}^{-1} \overline{\underline{KC}}^{-1} \underline{C}_P \ , \tag{6-1}$$

K denoting true covariances and C computational covariances as usual.

Let us split up this formula, using the method and the notations of (Moritz, 1973). We divide the observations $\underline{x}$ into two parts, the first part making up the vector $\underline{x}_1$, and the second part forming the vector $\underline{x}_2$. Thus the observation vector is partitioned as follows:

$$\underline{x} = \begin{bmatrix} \underline{x}_1 \\ \\ \underline{x}_2 \end{bmatrix} . \tag{6-2}$$

Similarly we split up the covariance matrices:

$$\bar{\underline{C}} = \begin{bmatrix} \underline{C}_{11} & \underline{C}_{12} \\ \underline{C}_{21} & \underline{C}_{22} \end{bmatrix} , \qquad \bar{\underline{K}} = \begin{bmatrix} \underline{K}_{11} & \underline{K}_{12} \\ \underline{K}_{21} & \underline{K}_{22} \end{bmatrix} , \tag{6-3}$$

$$\underline{C}_P = \begin{bmatrix} \underline{C}_{1P} \\ \underline{C}_{2P} \end{bmatrix} , \qquad \underline{K}_P = \begin{bmatrix} \underline{K}_{1P} \\ \underline{K}_{2P} \end{bmatrix} , \tag{6-4}$$

$$\underline{C}_P^T = \begin{bmatrix} \underline{C}_{P1} & \underline{C}_{P2} \end{bmatrix} \qquad \underline{K}_P^T = \begin{bmatrix} \underline{K}_{P1} & \underline{K}_{P2} \end{bmatrix} ; \tag{6-5}$$

for instance, $\underline{C}_{11}$ and $\underline{K}_{11}$ are covariance matrices for the vector $\underline{x}_1$. It is clear that

$$\underline{C}_{21} = \underline{C}_{12}^T , \qquad \underline{K}_{21} = \underline{K}_{12}^T ; \tag{6-6}$$

$$\underline{C}_{Pi} = \underline{C}_{iP}^T , \qquad \underline{K}_{Pi} = \underline{K}_{Pi}^T \quad (i = 1,2) . \tag{6-7}$$

The inverse matrix $\bar{\underline{C}}^{-1}$ is split up as follows:

$$\bar{\underline{C}}^{-1} = \begin{bmatrix} \underline{B}_{11} & \underline{B}_{12} \\ \underline{B}_{21} & \underline{B}_{22} \end{bmatrix} , \tag{6-8}$$

with the well-known relations (cf. Faddeeva, 1959, § 14):

$$\begin{aligned} \underline{B}_{22} &= (\underline{C}_{22} - \underline{C}_{21}\underline{C}_{11}^{-1}\underline{C}_{12})^{-1} , \\ \underline{B}_{12} &= -\underline{C}_{11}^{-1}\underline{C}_{12}\underline{B}_{22} , \qquad \underline{B}_{21} = -\underline{B}_{22}\underline{C}_{21}\underline{C}_{11}^{-1} , \\ \underline{B}_{11} &= \underline{C}_{11}^{-1} - \underline{C}_{11}^{-1}\underline{C}_{12}\underline{B}_{21} = \underline{C}_{11}^{-1} + \underline{C}_{11}^{-1}\underline{C}_{12}\underline{B}_{22}\underline{C}_{21}\underline{C}_{11}^{-1} . \end{aligned} \tag{6-9}$$

Using these relations we find:

$$\underline{C}_P^T\underline{C}^{-1}\underline{K}_P = \begin{bmatrix}\underline{C}_{P1} & \underline{C}_{P2}\end{bmatrix}\begin{bmatrix}\underline{B}_{11} & \underline{B}_{12}\\ \underline{B}_{21} & \underline{B}_{22}\end{bmatrix}\begin{bmatrix}\underline{K}_{1P}\\ \underline{K}_{2P}\end{bmatrix}$$

$$= \underline{C}_{P1}\underline{B}_{11}\underline{K}_{1P} + \underline{C}_{P1}\underline{B}_{12}\underline{K}_{2P} + \underline{C}_{P2}\underline{B}_{21}\underline{K}_{1P} + \underline{C}_{P2}\underline{B}_{22}\underline{K}_{2P}$$

$$= \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{1P} + (\underline{C}_{P2} - \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{C}_{12})\underline{B}_{22}(\underline{K}_{2P} - \underline{C}_{21}\underline{C}_{11}^{-1}\underline{K}_{1P}) \ . \tag{6-10}$$

With the abbreviations

$$\overline{\underline{C}}_{P2} = \underline{C}_{P2} - \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{C}_{12} \ , \quad \overline{\underline{C}}_{2P} = \underline{C}_{2P} - \underline{C}_{21}\underline{C}_{11}^{-1}\underline{C}_{1P} \ , \tag{6-11a}$$

$$\overline{\underline{K}}_{P2} = \underline{K}_{P2} - \underline{K}_{P1}\underline{C}_{11}^{-1}\underline{C}_{12} \ , \quad \overline{\underline{K}}_{2P} = \underline{K}_{2P} - \underline{C}_{21}\underline{C}_{11}^{-1}\underline{K}_{1P} \ , \tag{6-11b}$$

$$\overline{\underline{C}}_{22} = \underline{C}_{22} - \underline{C}_{21}\underline{C}_{11}^{-1}\underline{C}_{12} \ , \quad \overline{\underline{K}}_{22} = \underline{K}_{22} - \underline{C}_{21}\underline{C}_{11}^{-1}\underline{K}_{12} \ , \tag{6-12}$$

$$\overline{\underline{K}}_{12} = \underline{K}_{12} - \underline{K}_{11}\underline{C}_{11}^{-1}\underline{C}_{12} \ , \quad \overline{\underline{K}}_{21} = \underline{K}_{21} - \underline{C}_{21}\underline{C}_{11}^{-1}\underline{K}_{11} \ , \tag{6-13}$$

eq. (6-10) takes the form

$$\underline{C}_P^T\underline{C}^{-1}\underline{K}_P = \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{1P} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{2P} \ . \tag{6-14}$$

The last term in (6-1) is more laborious to transform. We first get

$$\underline{C}_P^T\underline{C}^{-1}\overline{\underline{K}} = \begin{bmatrix}\underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{11} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{21} & \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{12} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{22}\end{bmatrix} , \tag{6-15}$$

in complete analogy to (6-14), $\underline{K}_{1P}$ being replaced by the row vector $\begin{bmatrix}\underline{K}_{11} & \underline{K}_{12}\end{bmatrix}$ and $\underline{K}_{2P}$ being replaced by $\begin{bmatrix}\underline{K}_{21} & \underline{K}_{22}\end{bmatrix}$. By means of (6-15) we now have

$$\underline{C}_P^T\overline{\underline{C}}^{-1}\overline{\underline{KC}}^{-1}\underline{C}_P =$$

$$= \left[\underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{11} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{21} \quad \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{12} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{22}\right] \begin{bmatrix} \underline{B}_{11} & \underline{B}_{12} \\ \underline{B}_{21} & \underline{B}_{22} \end{bmatrix} \begin{bmatrix} \underline{C}_{1P} \\ \underline{C}_{2P} \end{bmatrix},$$

$\overline{\underline{K}}_{21}$ and $\overline{\underline{K}}_{22}$ being defined by (6-12) and (6-13). This equation is, in turn, transformed in the same way as (6-10), with the result, corresponding to (6-14),

$$(\underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{11} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{21})\underline{C}_{11}^{-1}\underline{C}_{1P} +$$

$$+ \left[\underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{12} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{22} - (\underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{11} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{21})\underline{C}_{11}^{-1}\underline{C}_{12}\right]\overline{\underline{C}}_{22}^{-1}\overline{\underline{C}}_{2P} .$$

This is finally brought into the form

$$\begin{aligned} \underline{C}_P^T\overline{\underline{C}}^{-1}\overline{\underline{KC}}^{-1}\underline{C}_P = {} & \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{11}\underline{C}_{11}^{-1}\underline{C}_{1P} + \\ & + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}(\overline{\underline{K}}_{22} - \overline{\underline{K}}_{21}\underline{C}_{11}^{-1}\underline{C}_{12})\overline{\underline{C}}_{22}^{-1}\overline{\underline{C}}_{2P} + \\ & + 2\overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{21}\underline{C}_{11}^{-1}\underline{C}_{1P} . \end{aligned} \tag{6-16}$$

By means of (6-14) and (6-16) we now obtain from (6-1):

$$m_{P,1}^2 = K_o - 2\underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{1P} + \underline{C}_{P1}\underline{C}_{11}^{-1}\underline{K}_{11}\underline{C}_{11}^{-1}\underline{C}_{1P} ; \tag{6-17}$$

$$\begin{aligned} m_P^2 = m_{P,1}^2 & - 2\overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{2P} + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{22}\overline{\underline{C}}_{22}^{-1}\overline{\underline{C}}_{2P} + \\ & + \overline{\underline{C}}_{P2}\overline{\underline{C}}_{22}^{-1}\overline{\underline{K}}_{21}\underline{C}_{11}^{-1}(2\underline{C}_{1P} - \underline{C}_{12}\overline{\underline{C}}_{22}^{-1}\overline{\underline{C}}_{2P}) . \end{aligned} \tag{6-18}$$

Here $m^2_{P,1}$ is the error variance (square of standard error) using the first part of the observations, which forms the vector $\underline{x}_1$, and m^2_P is the error variance using the complete observation vector (6-2). The barred quantities are defined by equations (6-11) to (6-13).

For the optimal estimation error, that is, if the computational covariances C coincide with the true covariances K , equations (6-17) and (6-18) become:

$$\hat{m}^2_{P1} = K_o - \underline{K}_{P1}\underline{K}^{-1}_{11}\underline{K}_{1P} , \qquad (6\text{-}19)$$

$$\hat{m}^2_{P} = \hat{m}^2_{P,1} - \underline{\bar{K}}_{P2}\underline{\bar{K}}^{-1}_{22}\underline{\bar{K}}_{2P} , \qquad (6\text{-}20)$$

in agreement with eq.(2-14) of (Moritz, 1973, p.11). Here the barred quantities are defined by equations (6-11) to (6-13), but with all C's replaced by the corresponding K's , so that, for instance, $\underline{\bar{K}}_{12}$ and $\underline{\bar{K}}_{21}$ are now zero.

Equations (6-17) and (6-18) are the basic result of this section; they will be used in the sequel.

7. Power Series Expressions for Interpolation Errors

To get a first idea on the influence of the choice of the covariance function in least-squares collocation, we consider the simple case of interpolation between two points with and without the use of gradients.

More precisely, we take the following case (Fig. 7-1). Let the two given stations P_1 and P_2

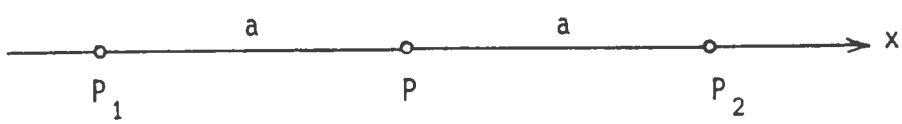

Figure 7-1

be at a distance of $2a$ apart, and let the interpolation point P be midway between the two stations P_1 and P_2. Let the x-axis pass through these three points.

As data we assume the gravity anomalies Δg and their horizontal derivatives $G \overset{\text{def}}{=} \partial \Delta g / \partial x$. (Essentially, $\Delta g = T_z$ and $G = T_{zx} = T_{xz}$, so that this case is basically the same as the case T_x, T_{xz} considered in (Moritz, 1975, p.53).) Thus the components of the observation vector $\underline{x}$ are

$$
\begin{aligned}
x_1 &= \Delta g_1 = \Delta g \quad \text{at} \quad P_1 \ , \\
x_2 &= \Delta g_2 = \Delta g \quad \text{at} \quad P_2 \ , \\
x_3 &= G_1 = \frac{\partial \Delta g}{\partial x} \quad \text{at} \quad P_1 \ , \\
x_4 &= G_2 = \frac{\partial \Delta g}{\partial x} \quad \text{at} \quad P_2 \ .
\end{aligned} \tag{7-1}
$$

We assume errorless data (no noise).

Let the covariance function of Δg be denoted by $C(s)$. Then, if A and B designate any two points of the set P_1 , P_2 , P , we have

$$\mathrm{cov}(\Delta g_A, \Delta g_B) = C(s) \ , \tag{7-2}$$

$$\mathrm{cov}(G_A, \Delta g_B) = \frac{\partial C}{\partial x_A} = -\,C'(s) \ , \tag{7-3}$$

$$\mathrm{cov}(\Delta g_A, G_B) = \frac{\partial C}{\partial x_B} = C'(s) \ , \tag{7-4}$$

$$\mathrm{cov}(G_A, G_B) = \frac{\partial^2 C}{\partial x_A \partial x_B} = -\,C''(s) \ , \tag{7-5}$$

where

$$s = x_B - x_A \ , \tag{7-6}$$

so that

$$\frac{\partial s}{\partial x_B} = 1 \ , \quad \frac{\partial s}{\partial x_A} = -\,1 \ .$$

The signal s_P to be estimated is Δg_P , that is, Δg at point P . Then the covariances (5-3) become:

$$
\begin{aligned}
C_{P1} &= \operatorname{cov}(\Delta g_P, \Delta g_1) = C(a) \ , \\
C_{P2} &= \operatorname{cov}(\Delta g_P, \Delta g_2) = C(a) \ , \\
C_{P3} &= \operatorname{cov}(\Delta g_P, G_1) = \operatorname{cov}(G_1, \Delta g_P) = - C'(a) \ , \\
C_{P4} &= \operatorname{cov}(\Delta g_P, G_2) = C'(a) \ .
\end{aligned}
\tag{7-7}
$$

Since we have assumed errorless data, the quantities D_{ik} in (5-4) are zero, so that

$$\bar{C}_{ik} = \operatorname{cov}(x_i, x_k) = C_{ik} \tag{7-8}$$

where

$$
\begin{aligned}
C_{11} &= C(0) = C_{22} \ , \\
C_{12} &= C(2a) \ , \\
C_{13} &= C'(0) = 0 = C_{24} \ , \\
C_{14} &= C'(2a) = - C_{23} \ , \\
C_{33} &= - C''(0) = C_{44} \ , \\
C_{34} &= - C''(2a) \ .
\end{aligned}
\tag{7-9}
$$

Hence (5-2) takes the symmetric form

$$
\Delta g_P = \begin{bmatrix} C_{P1} & C_{P1} & C_{P3} & - C_{P3} \end{bmatrix} \cdot
\begin{bmatrix} C_{11} & C_{12} & 0 & C_{14} \\ C_{12} & C_{11} & -C_{14} & 0 \\ 0 & -C_{14} & C_{33} & C_{34} \\ C_{14} & 0 & C_{34} & C_{33} \end{bmatrix}^{-1}
\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \ .
\tag{7-10}
$$

Briefly this may be written as

$$\Delta g_P = \underline{C}_P^T \underline{C}^{-1} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} . \tag{7-11}$$

We now perform a trick. We interchange the points P_1 and P_2 and invert the direction of the x-axis . Then the new observation vector becomes

$$\begin{bmatrix} x_2 \\ x_1 \\ -x_4 \\ -x_3 \end{bmatrix} , \tag{7-12}$$

but the matrices $\underline{C}_P^T$ and $\bar{C}$ do not change at all. Therefore we have, corresponding to (7-11), also

$$\Delta g_P = \underline{C}_P^T \underline{C}^{-1} \begin{bmatrix} x_2 \\ x_1 \\ -x_4 \\ -x_3 \end{bmatrix} . \tag{7-13}$$

On adding (7-11) and (7-13) and dividing by 2 we obtain

$$\Delta g_P = \underline{C_P^T C}^{-1} \begin{bmatrix} (x_1+x_2)/2 \\ (x_1+x_2)/2 \\ (x_3-x_4)/2 \\ -(x_3-x_4)/2 \end{bmatrix} . \tag{7-14}$$

We thus see that Δg_P has the form

$$\Delta g_P = A\frac{x_1+x_2}{2} + B\frac{x_3-x_4}{2} , \tag{7-15}$$

with certain coefficients A and B .

We just have shown that the estimated value Δg_P may be expressed as a linear combination of the quantities

$$u = \frac{x_1+x_2}{2} , \tag{7-16}$$

$$v = \frac{x_3-x_4}{2} . \tag{7-17}$$

We may thus consider these quantities u and v as our new measurements, in terms of which the least-squares estimation may be written as

$$\Delta g_P = \begin{bmatrix} C_{Pu} & C_{Pv} \end{bmatrix} \begin{bmatrix} C_{uu} & C_{uv} \\ C_{uv} & C_{vv} \end{bmatrix}^{-1} \begin{bmatrix} u \\ v \end{bmatrix} . \tag{7-18}$$

In this way we have been able to reduce the number of observations from 4 to 2, and the covariance matrix to be inverted is now a 2x2 instead of a 4x4 matrix. It should be noted that this reduction has been possible through the use of symmetries; no approximations are involved, so that (7-18) is rigorously equivalent to (7-10).

The covariances are readily calculated. For instance, by (7-7), (7-9), (7-16) and (7-17),

$$C_{Pu} = \mathrm{cov}(\Delta g_P, u) =$$

$$= \frac{1}{2}\mathrm{cov}(\Delta g_P, x_1) + \frac{1}{2}\mathrm{cov}(\Delta g_P, x_2)$$

$$= \frac{1}{2}(C_{P1} + C_{P2}) = C_{P1} \;;$$

$$C_{uv} = \mathrm{cov}(u, v) =$$

$$= \mathrm{cov}\left(\frac{x_1 + x_2}{2}, \frac{x_3 - x_4}{2}\right) =$$

$$= \frac{1}{4}\mathrm{cov}(x_1, x_3) + \frac{1}{4}\mathrm{cov}(x_2, x_3) -$$

$$- \frac{1}{4}\mathrm{cov}(x_1, x_4) - \frac{1}{4}\mathrm{cov}(x_2, x_4) =$$

$$= \frac{1}{4}(C_{13} + C_{23} - C_{14} - C_{24}) = - \frac{1}{2}C_{14} \, .$$

In this way we obtain:

$$\begin{aligned} C_{Pu} &= C(a) \, , \\ C_{Pv} &= - C'(a) \, , \\ C_{uu} &= \frac{1}{2}C(0) + \frac{1}{2}C(2a) \, , \\ C_{uv} &= - \frac{1}{2}C'(2a) \, , \\ C_{vv} &= - \frac{1}{2}C''(0) + \frac{1}{2}C''(2a) \, . \end{aligned} \tag{7-19}$$

It would not be difficult now to directly evaluate the estimation formula (7-18), using the covariances

(7-19), as well as the corresponding expression of the standard error,(5-14). We shall, however, choose here and in the following section the approach through stepwise collocation, because this approach shows particularly well the improvement of accuracy through the additional use of gradients: In the first step we take only Δg itself, that is, x_1 and x_2, or u; whereas in the second step we take also gradient observations, that is, x_3 and x_4, or v.

Using u (first step) and v (second step), and looking at (7-18), we see that the "submatrices" C_{uu}, C_{uv} are in this case simply numbers. Therefore, the matrix equations (6-17) and (6-18) reduce to ordinary algebraic expressions:

$$m^2_{P,1} = K_o - 2C_{Pu}C^{-1}_{uu}K_{Pu} + C^2_{Pu}C^{-2}_{uu}K_{uu} , \tag{7-20}$$

$$\begin{aligned} m^2_P = m^2_{P,1} &- 2\bar{C}_{Pv}\bar{C}^{-1}_{vv}\bar{K}_{Pv} + \bar{C}^2_{Pv}\bar{C}^{-2}_{vv}\bar{K}_{vv} + \\ &+ \bar{C}_{Pv}\bar{C}^{-1}_{vv}\bar{K}_{uv}C^{-1}_{uu}(2C_{Pu} - C_{uv}\bar{C}^{-1}_{vv}\bar{C}_{Pv}) , \end{aligned} \tag{7-21}$$

where, by (6-11a,b), (6-12) and (6-13),

$$\bar{C}_{Pv} = C_{Pv} - A\ C_{Pu} , \tag{7-22a}$$

$$\bar{C}_{vv} = C_{vv} - A\ C_{uv} , \tag{7-22b}$$

$$\bar{K}_{Pv} = K_{Pv} - A\ K_{Pu} , \tag{7-23a}$$

$$\bar{K}_{uv} = K_{uv} - A\ K_{uu} , \tag{7-23b}$$

$$\bar{K}_{vv} = K_{vv} - A\ K_{uv} , \tag{7-23c}$$

and

$$A = \frac{C_{uv}}{C_{uu}} \quad . \tag{7-24}$$

The quantities K_{Pu} , K_{Pv} , K_{uu} , K_{uv} , K_{vv} are computed from the "true" covariance function $K(s)$ in precisely the same way as the corresponding quantities C_{Pu} , C_{Pv} etc. are computed from the "computational" covariance function $C(s)$, namely by (7-19); there is

$$K_o = K(0) \quad . \tag{7-25}$$

Taylor Series Expressions.- We shall now expand the covariance functions $C(s)$ and $K(s)$ into power series:

$$C(s) = 1 - \alpha s^2 + \beta s^4 - \gamma s^6 \ldots , \tag{7-26}$$

$$K(s) = 1 - \lambda s^2 + \mu s^4 + \nu s^6 \ldots ; \tag{7-27}$$

for the time being we assume $C_o = K_o = 1$. Differentiation gives

$$C'(s) = - 2\alpha s + 4\beta s^3 - 6\gamma s^5 \ldots , \tag{7-28}$$

$$C''(s) = - 2\alpha + 12\beta s^2 - 30\gamma s^4 \ldots , \tag{7-29}$$

and corresponding expressions for $K'(s)$ and $K''(s)$. Thus (7-19) becomes, disregarding higher-order terms,

$$C_{Pu} = 1 - \alpha a^2 + \beta a^4 \quad ,$$

$$C_{Pv} = - 2\alpha a + 4\beta a^3 \quad ,$$

$$C_{uu} = 1 - 2\alpha a^2 + 8\beta a^4 \ ,$$

$$C_{uv} = - 2\alpha a + 16\beta a^3 \ , \qquad (7\text{-}30)$$

$$C_{vv} = 24\beta a^2 \ ;$$

analogous expressions hold for the K's . We now can compute the quantities (7-22) and (7-23) and substitute them into (7-20) and (7-21). The calculations are very lengthy but straightforward. The terms of zero and second degree cancel; there remains for (7-20)

$$m^2_{P,1} = (\alpha^2 - 2\alpha\lambda + 6\mu)a^4 + O(a^6) \ , \qquad (7\text{-}31)$$

and for (7-21),

$$m^2_P = m^2_{P,1} + (-\alpha^2 + 2\alpha\lambda - 6\mu)a^4 + O(a^6) \ . \qquad (7\text{-}32)$$

From these two expressions we may draw interesting conclusions. Their addition gives

$$m^2_P = O(a^6) \ . \qquad (7\text{-}33)$$

Thus, whereas the interpolation error using Δg only is of the order $O(a^4)$, the additional use of horizontal gradients reduces it to $O(a^6)$; it thus becomes essentially smaller. This is true also with the use of a non-optimal covariance function C .

Let us now turn to $m^2_{P,1}$, corresponding to simple interpolation without the use of gradients, and investigate the effect of a non-optimal covariance function. In the optimal case, that is, for $C(s) = K(s)$, eq. (7-31) reduces to

$$\bar{m}^2_{P,1} = (-\lambda^2+6\mu)a^4 + O(a^6) \ , \qquad \textbf{(7-34)}$$

since here $\lambda = \alpha$, $\mu = \beta$. The difference between (7-32) and (7-34) is, disregarding $O(a^6)$,

$$m^2_{P,1} - \bar{m}^2_{P,1} = (\lambda-\alpha)^2 a^4 \geqq 0 \ , \qquad (7\text{-}35)$$

so that

$$m^2_{P,1} \geqq \bar{m}^2_{P,1}$$

as it should be, since the use of a "wrong" (non-optimal) covariance function diminishes the accuracy.

In (7-26) we have for simplicity assumed $C_o = K_o = 1$. At the end of sec. 5 we have already pointed out that the variance C_o does not have any effect on m^2_P . Only the "true" variance K_o counts. To get expressions for m^2_P for $K_o \neq 1$, we must simply correct the scale by multiplying (7-31) and similar expressions by K_o , obtaining, for instance,

$$m^2_{P,1} = K_o(\alpha^2-2\alpha\lambda+6\mu)a^4 + O(a^6) \ . \qquad (7\text{-}36)$$

We also recognize the role of positive definiteness for the covariance function: the condition (2-15) reads in the present notation

$$6\mu - \lambda^2 \geqq 0 \ ,$$

which is necessary to obtain a positive $\bar{m}^2_{P,1}$, by eq. (7-34). If the covariance function were not positive definite, one might obtain imaginary interpolation errors!

The preceding expressions show again the basic role of the coefficients of s^2 in $C(s)$ and $K(s)$ and hence of the curvature parameter as defined in sec. 3.

It need hardly be mentioned that these considerations are not restricted to the interpolation of gravity anomalies Δg ; they hold for arbitrary signals and their covariance functions.

8. Interpolation Errors with Gaussian Covariances

We shall again consider the interpolation problem of sec. 7, but this time evaluating the error of interpolation for the case that the covariance functions are Gaussian functions (2-26):

$$C(s) = C_o e^{-A^2 s^2} , \tag{8-1}$$

$$K(s) = K_o e^{-B^2 s^2} . \tag{8-2}$$

We recall the geometrical situation, as illustrated by Fig. 7-1: there are two stations P_1 and P_2 at a distance of 2a apart, and the interpolation point P is situated halfway between P_1 and P_2. The data are given at both stations P_1 and P_2, namely

either only gravity anomalies Δg_1 and Δg_2, or
both Δg_1, Δg_2 and horizontal gradients G_1, G_2.

If the x-axis passes through P_1, P, P_2, then the horizontal gradient is

$$G = \frac{\partial \Delta g}{\partial x} . \tag{8-3}$$

As we have seen in (Moritz, 1975), this gradient (essentially T_{xz}), is by far the most effective component of the gradient tensor as regards improvement of interpolation; see especially pp. 52 and 69 of that report. Therefore it is reasonable to limit ourselves here to the consideration of this component (8-3).

The formulas (7-1) through (7-25) apply again. The computational formulas are (7-19) through (7-24). To evaluate them for the covariance functions (8-1) and (8-2), we need their derivatives:

$$C'(s) = C_o e^{-A^2 s^2} (-2A^2 s) , \tag{8-4}$$

$$C''(s) = C_o e^{-A^2 s^2} (-2A^2 + 4A^4 s^2) , \tag{8-5}$$

and similarly for $K'(s)$ and $K''(s)$, with C_o and A replaced by K_o and B.

We take

$$C_o = K_o = 1000 \text{ mgal}^2 , \tag{8-6}$$

keeping in mind that C_o has no influence on the interpolation error and that K_o determines the scale of the prediction error in mgals: if K_o is replaced by $\overline{K}_o$, then all prediction errors simply to be multiplied by

$$\sqrt{\overline{K}_o / K_o} \; .$$

More essential are the parameters A and B, which are related to the correlation length ξ by (3-19):

$$\xi_C = \frac{1}{A}\sqrt{\ln 2} \quad , \tag{8-7}$$

$$\xi_K = \frac{1}{B}\sqrt{\ln 2} \quad ; \tag{8-8}$$

ξ_C and ξ_K denote, respectively, the correlation lengths of the functions (8-1) and (8-2).

We shall fix ξ_K for the "true" covariance function $K(s)$ to be

$$\xi_K = 50 \text{ km} \tag{8-9}$$

and vary ξ_C for the "computational" covariance function $C(s)$, taking successively

$$\xi_C = \begin{array}{r} 25 \text{ km} , \\ 40 \text{ km} , \\ 50 \text{ km} , \\ 60 \text{ km} , \\ 75 \text{ km} , \\ 100 \text{ km} . \end{array} \tag{8-10}$$

This corresponds to the following situation. The "true" covariance function is assumed to be a Gaussian function (8-2), but its parameters K_o and B are not known. So we perform the interpolation by a formal least-squares collocation using a "computational" covariance function (8-1) with assumed parameters C_o and A; instead of A we may also prescribe ξ_C in view of the relation (8-7). We now ask in which way the use of $C(s)$ instead of $K(s)$ deteriorates the interpolation accuracy.

The answer to this problem is provided by equations (7-20) and (7-21), together with (7-22), (7-23) and (7-24). The resulting standard errors of interpolation are given in Table 8-1, using Δg data only, and Table 8-2 using g together with horizontal gradients G.

A first glance at the two tables shows already that the use of second-order gradients G_1 and G_2, in addition to Δg_1 and Δg_2, essentially improves the interpolation accuracy.

As to the effect of a "wrong" covariance function, we see that, within a wide range of correlation lengths ξ_C, we get practically the same accuracy as with the optimal value $\xi_C = 50$ km (the latter gives, of course, the minimum interpolation error corresponding to $C(s) = K(s)$). This is especially true for ξ_C greater than 50 km, so that, in case of doubt, it may be better to select a ξ_C which is too large than one which is too small.

Table 8-1

Standard Errors of Interpolation Using Δg_1 and Δg_2 for Covariance Functions $C(s)$ with Different Correlation Lengths ξ_C . Unit : 1 mgal.

a \ ξ_C	25 km	40 km	50 km	60 km	75 km	100 km
10 km	2.3	1.3	1.2	1.3	1.3	1.4
20	4.9	5.0	4.9	5.0	5.1	5.2
30	15.2	10.6	10.6	10.6	10.7	10.8
40	25.1	17.6	17.2	17.2	17.2	17.2
50	29.7	23.9	23.0	23.2	23.4	23.4
60 km	31.2	27.9	27.1	27.5	28.4	28.6

Table 8-2

Standard Errors of Interpolation Using Δg_1 , Δg_2 , G_1 , G_2 for Covariance Functions $C(s)$ with Different Correlation Lengths ξ_C . Unit : 1 mgal.

a \ ξ_C	25 km	40 km	50 km	60 km	75 km	100 km
10 km	0.1	0.0	0.0	0.0	0.0	0.0
20	1.8	0.4	0.3	0.3	0.4	0.5
30	7.8	1.9	1.6	1.7	1.9	2.1
40	18.9	5.2	4.7	4.8	5.2	5.7
50	27.0	11.6	10.1	10.3	10.7	11.2
60 km	30.3	19.5	16.9	17.4	17.9	18.2

Tables 8-1 and 8-2 give, so to speak, the "true" standard interpolation errors if a non-optimal covariance function is used. Thus they express the actual accuracy obtainable with the use of a non-optimal covariance function for interpolation. They can, of course, be computed only if the true covariance function $K(s)$ is known.

Table 8-3

Apparent Standard Errors of Interpolation Using Δg_1 and Δg_2 for Covariance Functions $C(s)$ with Different Correlation Lengths ξ_C . Unit : 1 mgal.

a \ ξ_C	25 km	40 km	50 km	60 km	75 km	100 km
10 km	4.9	1.9	1.2	0.9	0.6	0.3
20	17.2	7.6	4.9	3.4	2.2	1.2
30	27.1	15.6	10.6	7.6	4.9	2.8
40	30.7	23.0	17.2	12.8	8.5	4.9
50	31.5	27.8	23.0	18.3	12.8	7.6
60 km	31.6	30.2	27.1	23.0	17.2	10.6

Table 8-4

Apparent Standard Errors of Interpolation Using Δg_1 , Δg_2 , G_1 , G_2 for Covariance Functions $C(s)$ with Different Correlation Lengths ξ_C . Unit : 1 mgal.

a \ ξ_C	25 km	40 km	50 km	60 km	75 km	100 km
10 km	0.3	0.0	0.0	0.0	0.0	0.0
20	4.7	0.8	0.3	0.2	0.1	0.0
30	16.9	3.7	1.6	0.8	0.3	0.1
40	27.2	10.1	4.7	2.4	1.0	0.3
50	30.8	18.6	10.1	5.4	2.4	0.8
60 km	31.5	25.4	16.9	10.1	4.7	1.6

If $K(s)$ is unknown, then one might try to calculate some kind of standard interpolation error using (5-16) with $K(s)$ replaced by $C(s)$, that is, the expression (5-19). The results will be called "apparent standard errors" and given in Tables 8-3 and 8-4. We again assume that $\xi_C = 50$ km is the true value, so that the corresponding colums are the same as in Tables 8-1 and 8-2, respectively.

In sharp contrast to the results of the first two tables, Tables 8-3 and 8-4 give, for $\xi_C \neq 50$ km , results that differ strongly from the true values for $\xi_C = 50$ km .

The difference between Tables 8-1 and 8-2 on the one hand, and Tables 8-3 and 8-4 on the other hand should be carefully kept in mind. The use of a non-optimal covariance function for interpolation by eq. (5-1) is perfectly legitimate, it only does not give minimum standard error $\hat{m}_P$. In this case, the proper way of calculating m_P is by (5-14), and Tables 8-1 and 8-2 correspond to this case. On the other hand, the use of (5-19) for accuracy computation, on which Tables 8-3 and 8-4 are based, is mathematically unjustified; the only reason for using (5-19) is that it involves only C(s) , but we see that it gives results that can be quite misleading.

The comparison of Tables 8-1 and 8-2 with Tables 8-3 and 8-4 confirms once more that the use of an incorrect covariance for interpolation does not greatly change the interpolated value, but that for calculating accuracies the very best available covariances should be used.

If for accuracy studies a good covariance function is not available, then some possible covariance functions might be taken into consideration and their effect on the accuracy studied by means of formulas such as (5-14). In this way one might hope to obtain, at least, reasonable bounds for the accuracy of the quantities that are to be computed.

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