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FINITE COVARIANCE FUNCTIONS

Abstract

Because of the full covariance matrices and the computer storage limitations the number of measurements which can be handled by the collocation method simultaneously, is limited. This paper presents a method to compute covariance functions with a finite support yielding sparse covariance matrices. The theoretical background is pointed out and, for the one- and two-dimensional case, special functions are developed which can be combined with the usually used covariance functions to get a "finite covariance function". Simulated examples to demonstrate the behaviour of different solution methods to solve these special, sparse covariance matrices supplement our investigations.

1. Introduction

In many branches of geodesy it is necessary to interpolate and to predict data which can be considered as samples of a stationary stochastic process. A frequently applied procedure is the collocation method, with the following relations between the measurement l_D in a data point and the unknowns x, s, and n,

$$l_D = Ax + s_D + n \,. \tag{1}$$

The measurement consists of a deterministic part Ax and a stochastic part $s_D + n$. In this paper we shall confine ourselves, without restriction of the generality, to the pure prediction case, where the deterministic part vanishes.

$$l_D = s_D + n \tag{2}$$

The stochastic part is split up into the systematic part s_D (signal) and the purely random part n (noise). The characteristic of these parts are fixed by their expectations and covariances.

$$E\{s_D\} = s \tag{3}$$

$$E\{n\} = 0 \tag{4}$$

If we introduce the total expectation (cf. H. Moritz, 1980, p. 100), as the expectation of the mean value over the whole area, we assume the relation

Bull. Géod. 61 (1987) pp. 331–347.

$$M\{s_D\} = O\ , \tag{5}$$

to hold, and define this mean value in such a way that the noise remains unchanged

$$M\{n\} = n\ . \tag{6}$$

The autocovariance of the signal part is therefore defined by

$$cov\{s_D, s_D\} = E\{M\{s_D s_D^T\}\} = M\{s_D s_D^T\}\ , \tag{7}$$

which is the mean value of the product of the function values of all possible point combinations. The autovariance of the noise is given by

$$cov\{n, n\} = E\{M\{nn^T\}\} = E\{nn^T\}\ , \tag{8}$$

and the cross-covariance is supposed to vanish,

$$cov\{n, s_D\} = E\{M\{ns_D^T\}\} = E\{n\, M\{s_D^T\}\} = O\ . \tag{9}$$

In the sense of an L2-norm, the best linear estimation of the signal part s at an arbitrary point can be computed by the well-known prediction formulas

$$\tilde{s} = cov\{s, s_D\}\{cov\{s_D, s_D\} + cov\{n, n\}\}^{-1} l_D \tag{10}$$

with the error covariance matrix

$$cov\{\tilde{s}, \tilde{s}\} = cov\{s, s\} - cov\{s, s_D\}\{cov\{s_D, s_D\} + cov\{n, n\}\}^{-1} cov\{s, s_D\}^T\ . \tag{11}$$

The entire prediction process is performed within the following steps :

– split off a deterministic part (trend) from the measurements to fulfil the assumption (5)

– compute the empirical covariance function (formula (7))

– approximate the empirical covariance function by an analytic model

– compute the global covariance matrix

$$(cov\{s_D, s_D\} + cov\{n, n\})$$

– solve equations (10) and (11).

The most time-consuming job is the computation of the covariance matrix and the solution of the linear system, where one has to take care of two things : the stability of the matrix, and the storage limitations. Concerning the first fact, attention must be paid to the spacing of the data points. A small data spacing compared with the correlation length leads to a near singular matrix and to numerical problems if the noise part is too small. One proposed possibility to overcome such a problem is to replace such a point cluster by representative data, e.g. a mean value, another is simply to ignore parts of the information. Both methods however suffer of the drawback that the available information is not fully exploited.

The second difficulty is, that the covariance matrix is a completely filled in

matrix and therefore, the number of measurements which can be processed simultaneously, is limited. If it is possible to use a covariance function with a finite support, the covariance matrix becomes sparse and the solution of large systems can be done by special algorithms. But we have to pay attention to the fact, that the covariance matrix must be positive definite and therefore, we have to require a positive definite covariance function. Otherwise it can happen, that the error variance of an estimated signal exceeds the variance or that the error variance becomes less than zero. This can be seen by investigating formula (11).

The first idea to get a finite function is to truncate the covariance function or to neglect small coefficients of the covariance matrix outside an arbitrarily chosen band. This is equivalent to a multiplication of the covariance function by a unit step function; however, this yields a not necessarily positive definite matrix, because the unit step function is not a positive definite function and the result of the multiplication of a positive definite function by a nonpositive definite function is not necessarily a positive definite function.

In the following we have to solve two problems :

because positive definite functions are rather rare, we should investigate the rules how to combine functions to get a wide spectrum of positive definite models; the second is to find positive definite functions which have only a finite support. First we have to examine the existence of such a finite positive definite function. If we want to operate not only on the surface of a compact body, but also in the outer space, assuming harmonicity, we meet the problem, that harmonicity and finite support exclude each other. This is a consequence of the Dirichlet operator which has an integral kernel with an everywhere positive, unlimited support, yielding an unlimited support function in outer space even if the function has finite support at the surface. Vice versa, finite functions in the outer space can fulfil the harmonicity condition only approximately (confer. P. Meissl, 1981).

But we have to restrict our attention to finite functions on an arbitrary surface for the one- and two-dimensional case in the plane. For finite functions on the sphere, the analysis has still to be performed.

2. Theoretical Aspects

A covariance function of a stationary process must fulfil the requirement of positive definitness. Therefore, we have to proove that the spectrum $H(T)$ of the function $h(t)$ has positive values only. For the one-dimensional case this computation can be done by the Fourier analysis of $h(t)$

$$H(T) = F\{h(t)\} = \int_{-\infty}^{\infty} h(t)\, e^{-iTt}\, dt \tag{12}$$

with the inverse process, the Fourier synthesis

$$h(t) = F^{-1}\{H(T)\} = \frac{1}{2\pi} \int_{-\infty}^{\infty} H(T)\, e^{itT}\, dT\ . \tag{13}$$

The positive definiteness of a function is preserved by

- multiplication with a scalar greater than zero

– addition of two positive definite functions

– multiplication of two positive definite functions

– convolution of two positive definite functions.

The first property is trivial, the second comes from the fact that the covariance of the sum of two independent processes is the sum of their covariances ($cov_{x+y} = cov_x + cov_y$), the third comes from the corresponding property of the product of two independent processes ($cov_{xy} = cov_x\, cov_y$), and the last comes from the fact that the product of two positive spectra is positive and from the convolution theorem. On the other hand, each convolution of a function with itself produces a positive definite function, because this corresponds to the multiplication of the spectrum with itself. Using this fact and solving the convolution for homogeneous functions,

$$g(t) = h(t) * h(t)$$

$$= \int_{-\infty}^{\infty} h(s)\, h(t-s)\, ds\ , \tag{14}$$

we are able to compute positive definite functions. According to the above mentioned rules these functions can be combined with other well-known positive definite functions, providing a lot of positive definite models.

In the two-dimensional case we use the fact, that the two-dimensional Fourier analysis and Fourier synthesis can be treated as two one-dimensional processes

$$H(X,Y) = F\left\{F\left\{h(x,y)\right\}_x\right\}_y \tag{15}$$

and

$$h(x,y) = F^{-1}\left\{F^{-1}\left\{H(X,Y)\right\}_X\right\}_Y\ . \tag{16}$$

Therefore all the rules of the one-dimensional case hold, and the two-dimensional convolution of a function with itself leads also to a multiplication of the spectrum with itself.

Now let us have a look to a practical example. First, we treat only the one-dimensional case, and afterwards we solve the problem for two dimensions. In both cases we use functions with a finite support and, employing the convolution theorem, derive positive definite functions, which have a finite support too. We call these functions "finite covariance functions".

2.1. Finite Covariance Functions in the One-dimensional Case

Let us begin with the simplest case. We make a convolution of the unit step function S0 (t) *(Fig. 1)*, which is defined by

$$S0(t) = \begin{cases} 1 \text{ for } |t| \le \dfrac{1}{2} \\ \\ 0 \text{ else} \end{cases} \tag{17}$$

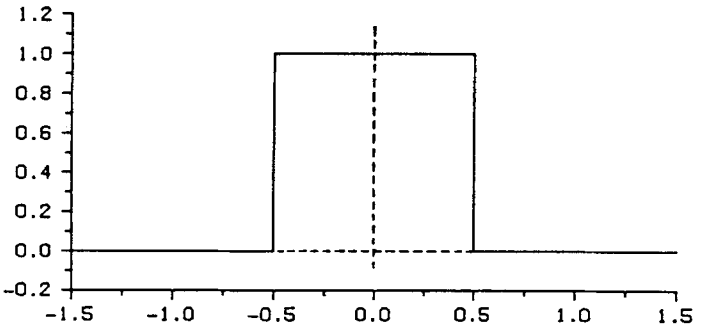

Fig. 1 — Unit step function

with itself, yielding

$$S1(t) = S0(t) * S0(t) , \tag{18}$$

$$S1(t) = \begin{cases} 1 - |t| & \text{for } |t| \; S1 \\ 0 & \text{else} \end{cases} \tag{19}$$

This function — the linear spline (Sünkel, 1984) function *(Fig. 2)* — is positive definite in the one-dimensional case; because of the discontinuity of the derivative at $t = 0 , \pm 1$ it is not a very useful function for our purposes.

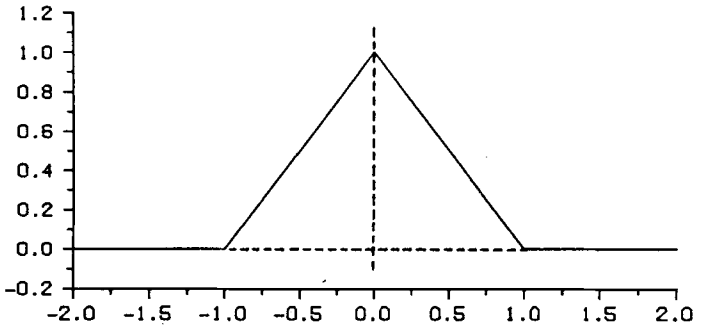

Fig. 2 — Linear spline function

We know (cf. H. Sünkel, 1981) that the result of the convolution of the linear spline function with itself yields the cubic spline function *(Fig. 3).* Since this comes from the convolution of a function with itself the result must be a positive definite function too.

$$S3(t) \quad \frac{1}{6} \begin{cases} 3|t|^3 - 6t^2 + 4 & \text{for} \quad |t| \leq 1 \\ (2-|t|)^3 & \text{for} \quad 1 \leq |t| \leq 2 \\ 0 & \text{else} \end{cases} \tag{20}$$

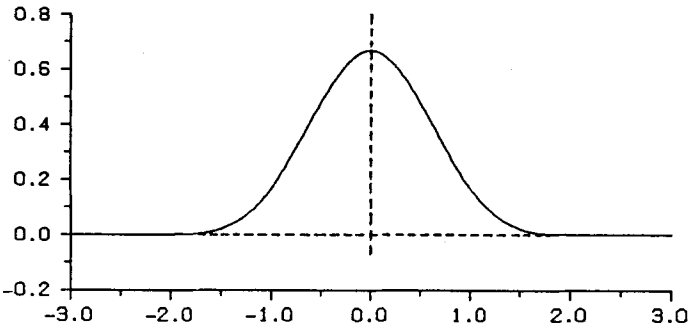

Fig. 3 – Cubic spline function

Consequently, each spline function which can be computed by a convolution with itself or by a convolution of two positive definite functions, is also positive definite (e.g. S1 , S3 , S5 , S7 ...) .

Combining these finite positive definite functions with one of the most used models of positive definite functions

$$e^{-a|t|}, \; e^{-at^2}, \; \frac{sin(at)}{at}, \; cos(at) \qquad a > 0 \; , \tag{21}$$

we gain a large variety of possible models to fit empirical covariance functions.

2.2. Finite Covariance Functions in the Two-dimensional Case

We start again with a simple example, convolving the following isotropic function (cylinder) with itself :

$$h(r) = \begin{cases} 1 & \text{for} \quad r \leq R = const. > 0 \\ 0 & \text{else} \end{cases} \tag{22}$$

For the general two-dimensional case the convolution of a homogeneous function with itself has the form

$$g(x,y) = \int_{-\infty}^{\infty}\int h(u,v)\, h(x-u, y-v)\, du\, dv \; . \tag{23}$$

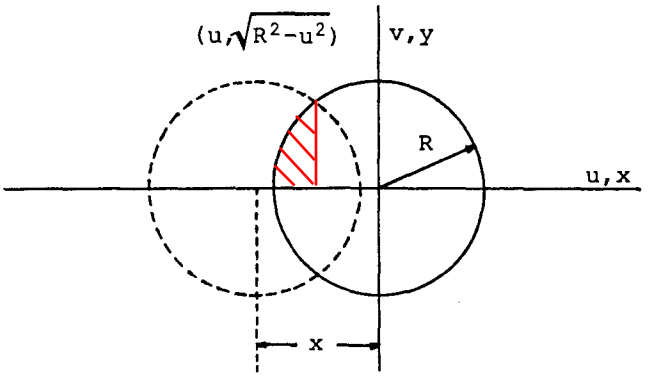

Fig. 4 — Convolution of a cylinder with itself

In the isotropic case we set the variable y to zero, change the variable x to $\bar{r}$, and get

$$g(\bar{r}) = \int_{-\infty}^{\infty}\int h(u,v)\, h(\bar{r}-u,v)\, du\, dv \ . \tag{24}$$

Inserting function (22) and changing the upper and lower limits appropriately we receive, because of the symmetry,

$$g(\bar{r}) = 4 \int_{\bar{r}/2}^{R} \int_{0}^{\sqrt{R^2-u^2}} dv\, du \ . \tag{25}$$

If we solve this system we obtain

$$g(\bar{r}) = \begin{cases} 2R^2\, arcos\left(\dfrac{\bar{r}}{2R}\right) - \bar{r}\sqrt{R^2-\left(\dfrac{\bar{r}^2}{2}\right)} & \text{for } \bar{r} \leq 2R \\ 0 & \text{else} \end{cases} \tag{26}$$

This function is not continuously differentiable; therefore, it doesn't lend itself for application.

We try to solve the more complicated case of the convolution of a parabolic function (27) with itself.

$$h(r) = \begin{cases} R^2 - r^2 & \text{for } r \leq R = const. > 0 \\ 0 & \text{else} \end{cases} \tag{27}$$

We use the same bounds as before and we are able to write down the convolution in the following way

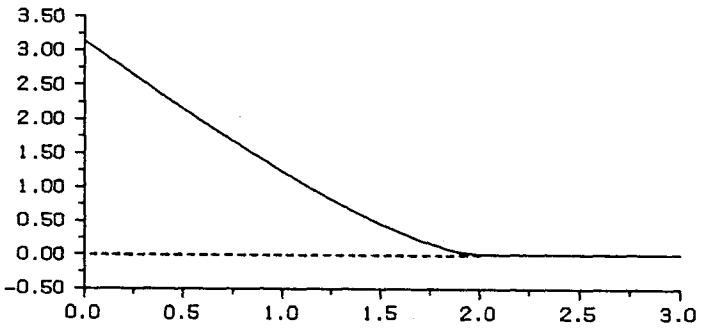

Fig. 5 – Graph of the function (26)

$$g(\bar{r}) = 4 \int_{\bar{r}/2}^{R} \int_{0}^{\sqrt{R^2-u^2}} (R^2 - (\bar{r}-u)^2 - v^2)\,(R^2 - u^2 - v^2)\,dv\,du \,. \qquad (28)$$

After reorganizing this equation and performing one integration we obtain

$$g(\bar{r}) = \frac{4}{15} \int_{\bar{r}/2}^{R} [\,8u^4 - 20\bar{r}u^3 + (10\bar{r}^2 - 16R^2)\,u^2 + 20R^2\,\bar{r}u -$$

$$- 10R^2\,\bar{r}^2 + 8R^4\,]\,\sqrt{R^2-u^2}\,du \,. \qquad (29)$$

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In this equation all integrands are of the type

$$u^n \sqrt{R^2-u^2}\,;$$

its integral can be found in any mathematical textbook (e,g, I. Bronstein, 1973; p. 424) or solved by substitution with the trigonometric functions *sine* and *cosine*. Finally we obtain

$$g(\bar{r}) \begin{cases} \frac{1}{3}R^6\,\pi - \frac{1}{2}R^4\,\bar{r}^2\,\pi + \\ \quad + \frac{1}{3}\left(R^4\,\bar{r} + \frac{4}{3}R^2\,\bar{r}^3 - \frac{1}{12}\bar{r}^5\right)\sqrt{R^2 - \left(\frac{\bar{r}}{2}\right)^2} + \\ \quad + (R^4\,\bar{r}^2 - \frac{2}{3}R^6)\,\arcsin\,\frac{\bar{r}}{2R} \quad \text{for} \quad r \leq 2R \\ 0 \qquad\qquad\qquad\qquad\qquad\qquad \text{else} \end{cases} \qquad (30)$$

The graphical representation looks like :

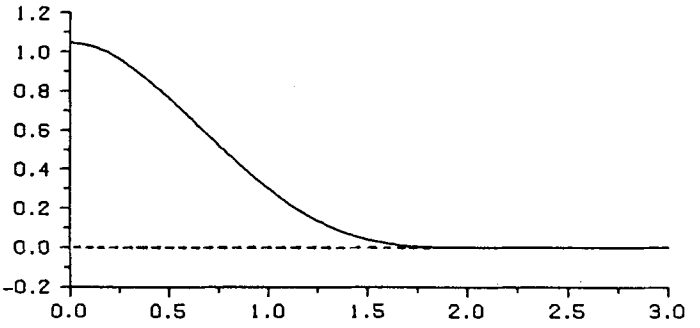

Fig. 6 — Graph of the function (30)

This function is continuous and continuously differentiable over the whole plane. As we mentioned before, the possibility of combining these finite functions with other well-known positive definite two-dimensional functions like

$$e^{-ar},\ e^{-ar^2},\ J_0(ar),\ \frac{J_1(ar)}{ar},\qquad a>0 \quad r>0 \tag{31}$$

(J_0, J_1 ... Bessel functions of the first kind) provides much freedom in fitting the empirical covariance functions by analytical models.

3. Numerical Experiments

To study the numerical behaviour of the sparse covariance matrix derived from the finite covariance function, an analytical surface model is used which consists of a linear combination of *sine* and *cosine* functions

$$f(x,y) = A \sum_{i=1}^{n} a_i \sin\left(\beta_i \frac{2\pi}{L} x + \gamma_i\right) \cos\ \delta_i \frac{2\pi}{L} y + \epsilon_i \tag{32}$$

with the $5n+2$ parameters $\{a_i, \beta_i, \gamma_i, \delta_i, \epsilon_i\}$, A, L.

In the following examples we have chosen $n=3$ (which corresponds to 17 parameters) and got the reference surface shown in *Fig. 7.* This surface was digitized on a square grid with 11×11 points. The contours are generated by the software system GSPP, written by H. Sünkel, 1980.

Fig. 7 shows also 25 data points which are used as sample points for an approximation of this surface by the prediction algorithm. According to chapter 1 we should remove from our data the deterministic part — called trend — to fulfill the assumption (5). For our example the trend is shown in *Fig. 8* (cubic polynomial model). With the remaining part we compute the empirical covariance function (see *Table 1,* columns 2 and 3) and, because of the small number of data points, a moving average

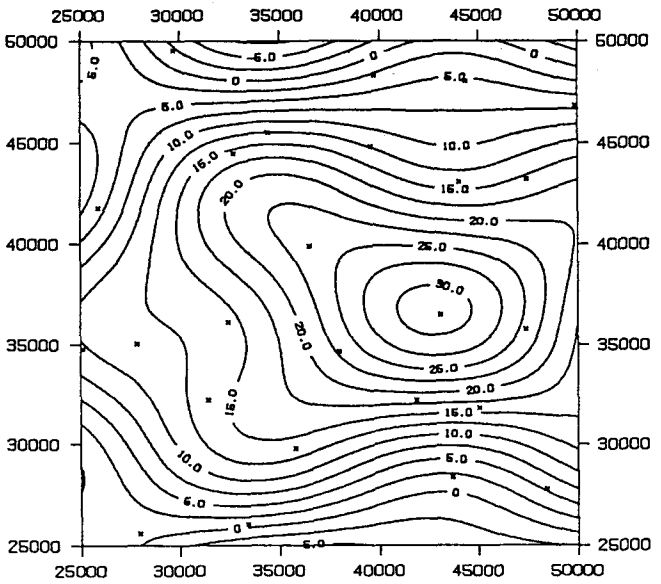

Fig. 7 — Reference surface with 25 data points

(Table 1, columns 4 and 5*).* This function has to be approximated by an analytical model.

For comparison purposes we present two analytical models, one with an infinite support (33) and one with a finite support of 18.000 units (34). *Cf. Table 1.*

$$(\text{model 1})\ cov\,(r) = a\,e^{-b\,r^2}\,J_0\,(cr) \qquad a, b, c > 0 \ \ldots\ const. \tag{33}$$

$$(\text{model 2})\ cov\,(r) = g\,(r)\,a\,J_0\,(cr) \qquad a, c > 0 \quad \ldots\ const. \tag{34}$$

$g\,(r)$ ... finite covariance function (30)

($J_0\,(r)$ = Bessel's function of order 0)

The corresponding solutions of the prediction are shown in *Fig. 9* and *Fig. 10.*

The main advantage of the solution with a finite covariance function is the sparseness of the covariance matrix. To solve such sparse matrices there exist a number of algorithms. In many numerical tests the profile (variable bandwidth) algorithm and the conjugate gradient (cg) method proved to be the best solution methods for such problems. To demonstrate the behaviour of these solution methods we made some simulations.

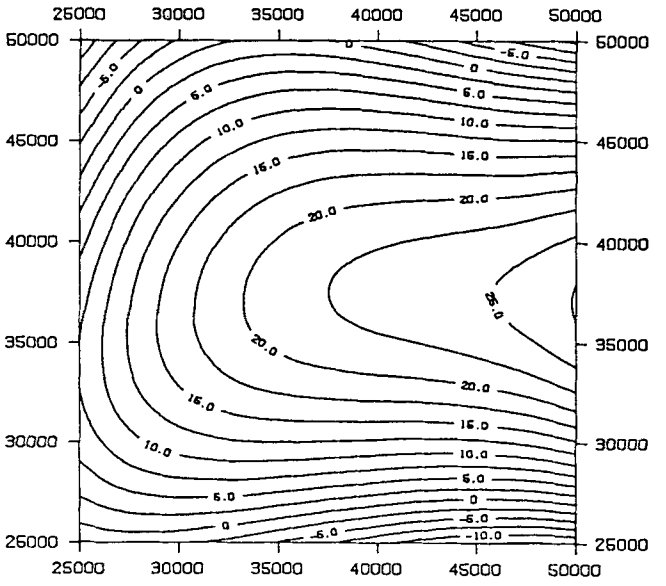

Fig. 8 — Deterministic part (cubic polynomial model)

Table 1

Empirical and analytical covariance functions

dist.	number of data pairs	empir. covariance	number of data pairs	empir. covariance	anal. model 1	anal. model 2
0	25	6.706	25	6.706	6.597	6.597
1000	1	2.770	6	2.901	6.230	6.130
3000	5	3.162	37	2.077	3.663	3.202
5000	31	−0.785	57	−0.153	0.184	0.129
7000	21	−2.202	82	−2.104	−2.123	−1.070
9000	30	−3.227	88	−2.306	−2.220	−0.705
11000	37	−0.568	99	−0.541	−0.684	−0.113
13000	32	2.201	105	1.155	0.962	0.061
15000	36	0.784	99	1.056	1.496	0.020
17000	31	0.456	93	0.217	0.801	0.000
19000	26	−0.828	76	−0.458	−0.307	
21000	19	−0.632	63	−0.499	−0.909	
23000	18	0.095	43	0.013	−0.690	
25000	6	0.492	29	0.402	−0.029	
27000	5	0.530	12	0.117	0.468	
29000	1	−1.084	6	−0.546	0.484	

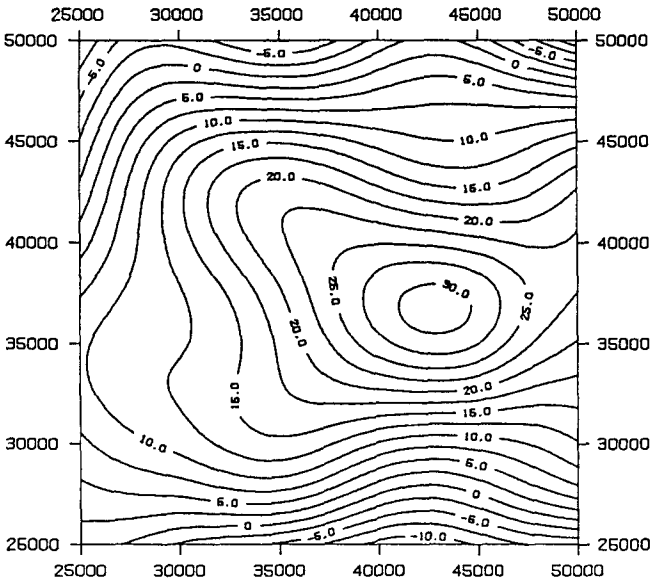

Fig. 9 – Prediction with infinite support

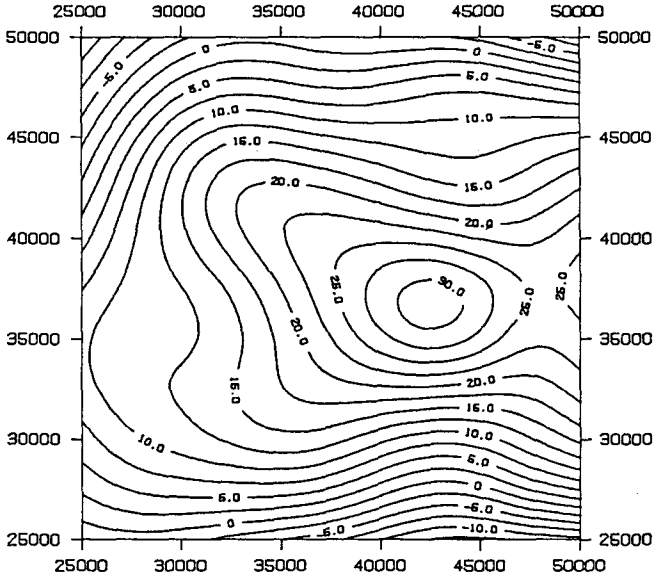

Fig. 10 – Prediction with finite support

Of main interest is the influence of different supports of the finite covariance function on the storage and CPU-time requirement. Also the increase of effort with an increasing number of data points has to be studied. To show these effects we executed three groups of simulations :

The first group is characterized by a constant area of investigation (25000 x 25000) using a constant number of data points (400), but changing the support of the finite covariance function. *Fig. 11* shows the storage requirement and demonstrates the behaviour of the CPU-time needed to set up the covariance matrix and to solve the linear system using the profile algorithm and the conjugate gradient algorithm, respectively. All the computations are performed on a VAX 725 without an arithmetic processor. Our intention is to desmonstrate the behaviour of the solution time and not the absolute values. Because of the influence of the noise on the conjugate gradients, two different computations are performed : one without noise and one with a ratio of 0.1 between $cov\{n, n\}$ and $cov\{s, s\}$ $[cov\{n, n\}/cov\{s, s\} = 0.1]$.

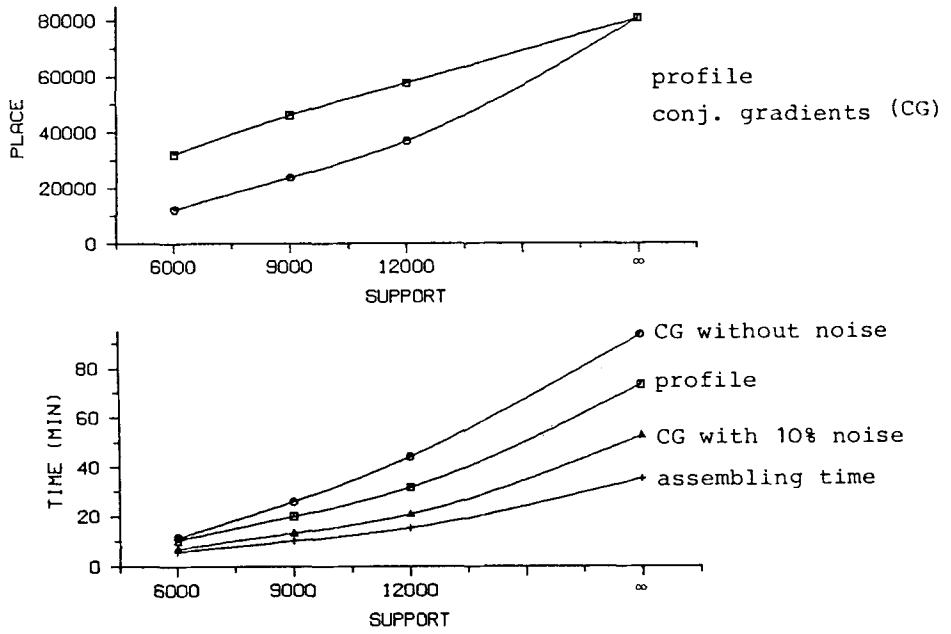

Fig. 11 — Storage and CPU—time requirement with area const. and number of points const.

In the next group of simulations the area is kept constant (25000 x 25000), but the number of points increases and therefore, the point density grows; the support is constant (6000). In *Fig. 12* required storage and CPU-time are shown.

The third simulation group is characterized by a constant point density (1 point/1000 x 1000) and a constant support (6000), but the number of points and the extension of the area varies (cf. *Fig. 13)*.

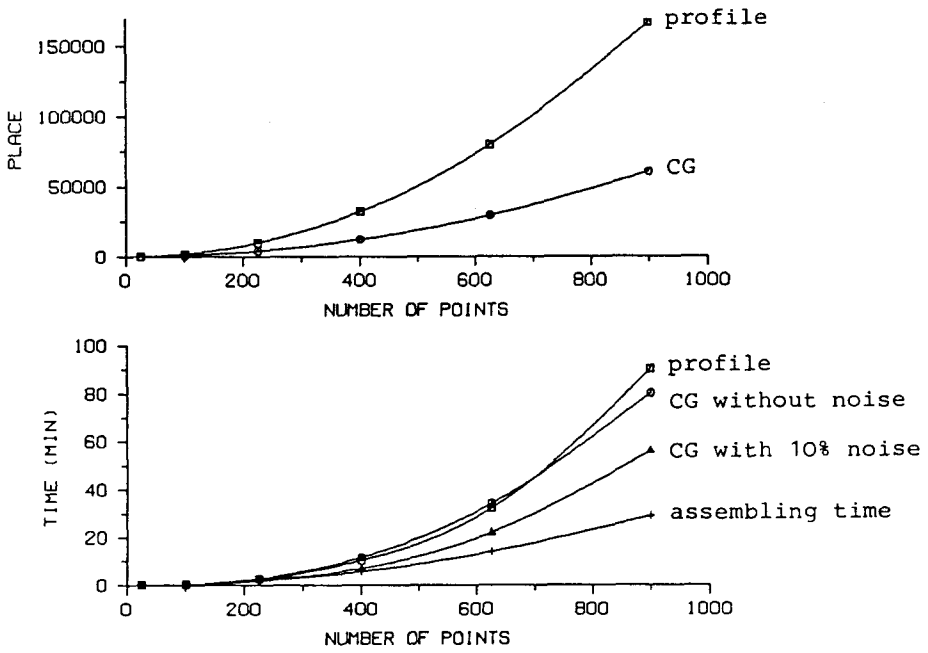

Fig. 12 – Storage and CPU–time requirement with area const. and support const.

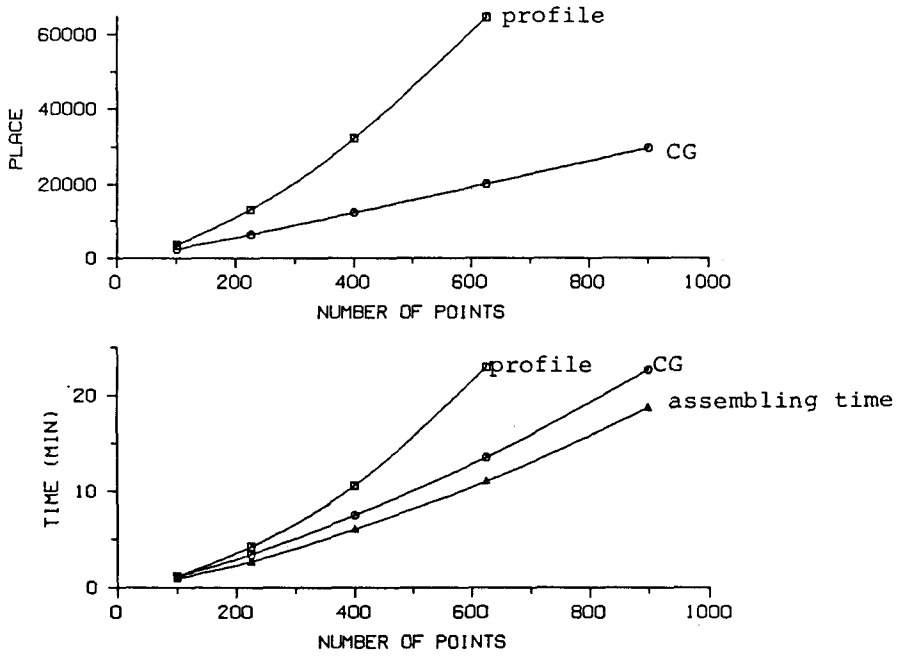

Fig. 13 – Storage and CPU–time requirement with point density const. and support const.

Let us now discuss the results. The storage requirement for the profile algorithm is proportional both to the number of points and the mean bandwidth. The mean bandwidth depends linearly on the support of the finite function and, if we assume a square-size area, on the square root of the number of points. Therefore the required storage is proportional to $n\sqrt{n}\ s$ (n ... number of points, s ... support). The expected solution time is of the order of the product of the number of points and the square of the mean bandwidth (cf. R.H. Hanson, 1978; p. 429); in a square area it is $n^2\ s^2$. The influence of the support of the finite function is quadratic, because the bandwidth grows linearly with increasing support.

Judging from ***Figures 11, 12,*** and ***13*** the storage requirement for the conjugate gradient method depends only linearly on the number of points and quadratically on the support because, if the support becomes larger, the number of nonzero covariance elements grows quadratically. The solution time is affected by the ratio of $cov\{n, n\}/cov\{s, s\}$. With a small noise part the solution time comes close to the solution time of the profile algorithm. In the case that the ratio $cov\{n, n\}/cov\{s, s\}$ is close to 0.1, the conjugate gradients work much faster than the profile algorithm. If the point density and the support is constant (cf. ***Fig. 13***), the number of iterations becomes constant – because the size of the eigenvalues is nearly independent of the extension of the area – and the solution time grows only linearly with the number of unknowns.

4. Discussion and conclusions

Before coming to some conclusions on the work presented in this paper, the authors, also compelled by the reviewers to whom they are grateful, would like to open a brief discussion on the assumptions underlaying the actual presentation.

In our feeling the main assumptions are the following two :

– that the principle leading to the estimation formula (10) is quite robust with respect to the use of the "true" signal covariance function, in particular also considering that the same formulas can be derived in a deterministic context from a minimum hybrid norm principle (cf. Sansò, 1986);

– that according to the practice (cf. Sansò, 1985) of anybody experienced with covariance modelling, we know that the tail of the empirical covariance function is very poorly estimated so that we can model these values more according to general requirements, than with respect to the empirical values.

The first assumption yields an interpolator of the form (10) with a matrix $C = cov\{s_D, s_D\}$ necessarily positive finite (in the deterministic interpretation this is related to the matrix chosen to express the minimum norm principle) : the second assumption implies that we are free to send to zero the model covariance function, with the gain in the computation of formula (10) that is illustrated in this work.

Obviously both principles can be criticized or used in a different way.

Starting from the latter, for instance, we can maintain that taking a usual covariance model and truncating it at a suitable distance can provide a simple and good covariance model. Naturally we know that the risk is to get a non positive-function but in practice many times the normal matrix is still positive definite if the truncation value is fairly large.

As for the first point, we must admit that the positive definiteness of the "covariance function" could also be questioned and solutions with non positive functions could be proposed.

We must say that the reasons to use positive definite functions are from our view-point, superior.

In fact :

– a positive covariance function is strictly related to the theory of minimizing quadratic functionals,

– it gives rise to an always well posed numerical problem (if some noise is present $\sigma_n^2 \neq 0$) in the inversion of the normal matrix,

– it allows for a meaningful expression of the estimation error, where no "error variance" is negative.

Nevertheless the idea of studying the effect of the use of non positive definite covariance function in terms of the estimation error is interesting, and we plan to discuss this in another paper for a simple example of filtering, where we can take advantage of the spectral representation.

Concluding, we can say that the method presented above of modelling covariance functions by combining a positive definite function with one of finite support function is a very powerful tool and makes the prediction method attractive, even for a very large number of data.

This method doesn't need much storage; for large areas the storage and CPU-time requirement grow only linearly (cf. *Fig. 13*). These features make this interpolation method (finite covariance function – conjugate gradients) superior to all other methods known to the authors.

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Received : 01.04.1987
Accepted : 05.10.1987