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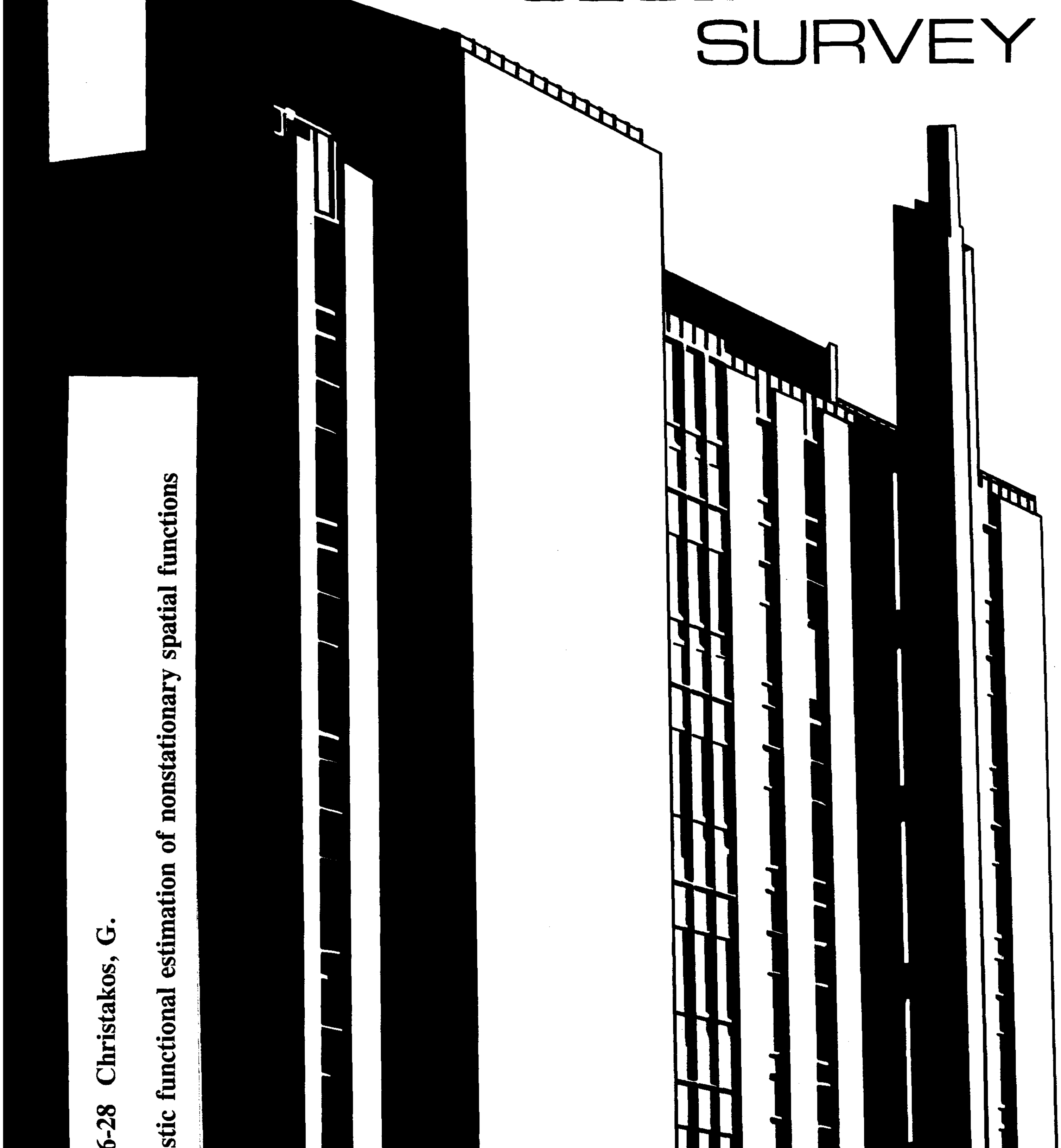

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NON-STOCHASTIC FUNCTIONAL ESTIMATION OF NONSTATIONARY SPATIAL FUNCTIONS

George Christakos

Kansas Geological Survey

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George Christakos
Kansas Geological Survey
1930 Constant Ave., Campus West
University of Kansas
Lawrence, KS 66046

Abstract

A non-stochastic approach of modelling and estimating linear functionals of nonstationary spatial functions is presented. The concept is applicable to multidimensional phenomena characterized by the hypothesis of inherentity: the originally nonstationary function has spatially stationary increments of some order. Working within a purely non-stochastic framework, an attempt is made to surmount theoretical and practical restrictions of the standard stochastic treatment of multimensional data, leading to several interesting mathematics. The model is conceptually completely different from the classical stochastic methodology. It is interesting however, that certain of the results obtained are formally identical with these of the latter.

Key words: Non-stochastic optimization, spatial functions.

1. Introduction

This work deals with the following problem: If the values of a spatial function are known at a number of points, we seek the optimal estimation of the value of the function, or in general of any linear functional of the function, at any point in space. Problems of this type occur frequently in physical and social sciences. Examples include contour and grid mapping of seismic parameters, the variation of the specific gravity of shale oil in a deposit, or the employment levels of a country at census points.

Such situations may be investigated by means of the theory of random fields or functions (Wiener [1] Yaglom [2], Matheron [3], Schagen [4]), but there are conceptual difficulties inherent in the stochastic approach and, also, practical difficulties due to the possible nonstationarity of the real data. The conceptual difficulties stem from the fact that we usually have only one data record which, in the stochastic way of thinking, is one sample from the collection of all possible records. The practical difficulties are related to the evaluation of the stochastic correlation structure of the random field when the observed phenomenon exhibits a certain statistical irregularity.

On the other hand, traditional deterministic methods like least squares, polynomial interpolation or weighted coefficients (Rice [5], Meinardus [6], Davis [7]) have several disadvantages when used to solve the above optimization problem. For example, they do not provide an assessment of the accuracy of the functional estimation and they may lead to unrealistic estimates when the spatial variability of the function is not sufficiently regular.

This presentation is an attempt to avoid the purely stochastic approaches without losing their important features such as information on the functional estimator's accuracy. Moreover, we will study the possible irregularities of the real data by introducing the non-stochastic notion of inherent spatial functions. The latter is an interesting class of spatial functions which are, in general, nonstationary but they have stationary increments of some order. Then, the object under study is no longer the nonstationary function but rather our attention is focused on these increments which have computable correlation structure. In particular, section 2 provides a rigorous statement of the optimization problem assuming linear functionals and functional estimators. In sections 3 and 4 we specify the class of inherent spatial functions for which the optimization is carried out. Intuitively, inherentity may be viewed as an extension to multidimensional spaces and arbitrary data patterns of the Box-Jenkins approach (which eliminates the polynomial components of nonstationary time-series, Box and Jenkins [8]). However, the difficulties that arise in the multidimensional setting are qualitatively different to those handled by the one dimensional theory. Furthermore, from a strictly mathematical standpoint, both the inherent function and its increments are introduced in a well established deterministic sense with no resort to stochastic concepts. In section 5, we look at the solution of the optimization problem based on the assumptions and the theoretical results of the preceding sections. This leads to an optimal estimator with several interesting properties, for example, it gives the measured values at the data points and is, therefore a perfect interpolator. Finally, a computational procedure is established in section 6, where we also discuss a numerical application.

2. Formulation of the problem

In this study, we consider a class of optimization problems which are of the following general type (Problem P).

<u>Problem P</u>: Let x_i, $i = 1,2,\ldots,N$, be N distinct points in R^n, where measurements of an unknown spatial, in general nonstationary, function f(x) are available. We seek the optimal estimation of the linear functional

$$\Psi[f] = \int_F f(x)\,\Psi(dx) \tag{1}$$

defined on some support F over which the measure $\Psi(dx)$ is nonnegative.

Here we should point out that the nonstationarity of the spatial function f(x), as it is considered throughout the paper, implies by definition that the limit

$$\langle f(x),\, f(x+h)\rangle = \lim_{V \to R^n} \frac{1}{V} \int_V f(x)\, f(x+h)\, dx \tag{2}$$

may not exist for some $h \in V$. As a consequence the correlation structure of f(x) cannot be expressed via the convolution (2), as in the case of stationarity when the limit (2) does exist. We are primarily concerned with functionals for which the linear relationship is true, i.e.

$$\Psi[\sum_i \mu_i f_i] = \sum_i \mu_i \Psi[f_i] \tag{3}$$

where $\mu_i \in R^n$. Typical examples are, the point-functional

$$\Psi[f] = f(x) \tag{3a}$$

and the volume-functional

$$\Psi[f] = \int_V f(x)\, dx \tag{3b}$$

The corresponding measures $\Psi(dx)$ will be, respectively,

$\Psi(dx)=dx\ \delta(x-x')$, where δ is the dirac-measure, and

$\Psi(dx)=dx$ if $x \in V$, $= 0$ if $x \notin V$.

Other interesting functionals include differentiation and convolution.

Of course, in its present form Problem P is not a completely defined problem. It will be now restated as a constrained optimization problem; more specifically,

Problem P_o: Solve Problem P so that the optimal estimator $\hat{\Psi}[f]$ of the functional $\Psi[f]$ satisfies the conditions below:

C1) It is linear-form, i.e.

$$\hat{\Psi}[f] = \sum_i \xi_i\ f(x_i) \tag{4a}$$

where $\xi_i \in R$ and $x \in S$, where S is a subset of the data points.

C2) It is location-invariant, i.e.

$$\hat{\Psi}[f(x+x')] = \sum_i \xi_i\ f(x_i + x') \tag{4b}$$

for all $x' \in R^n$.

C3) It minimizes the mean square estimation error, i.e.

$$\langle\{\hat{\Psi}[f] - \Psi[f]\}^2\rangle = \lim_{V \to R^n} \frac{1}{V} \int_V \{\hat{\Psi}[f(x+x')] - \Psi[f(x+x')]\}^2 dx'$$
$$= \text{minimum} \qquad (4c)$$

subject to the constraint

$$\langle\hat{\Psi}[f] - \Psi[f]\rangle = \lim_{V \to R^n} \frac{1}{V} \int_V \{\hat{\Psi}[f(x+x')] - \Psi[f(x+x')]\} dx' \qquad (4d)$$
$$= 0$$

where the functionals may take one of the forms discussed above (equ(3a), (3b), etc).

Still, Problerm P_o seems to be not completely defined, since the function f is unknown. However there can be introduced certain asumptions regarding the structure of function f which will make it a well-posed problem. But we postpone discussion of these until a detailed account of the spatial model has been given. Nevertheless, it is clear that one should work with functions for which finite values are computed for the above quantities. Due to the possible nonexistence of the limit (2), instead of focusing attention on the nonstationary function f(x), one may instead concentrate on an incremental function resulting from f(x) with the aid of some well defined operations. The solution of the Problem P_o is then reduced to the determination of the coefficients ξ_i of equ (4a) so that conditions (4c) and (4d) are satisfied. From equ (4b) we see that these coefficients are invariant to any translation where the vector distances between the data points and the support F, and also between the data points themselves, do not change. However, in order to include possible anisotropies, such an invariance is not assumed to be valid for rotations.

3. Incremental functions and related topics.

Associated with the optimization theory developed in this presentation, is the important concept of incremental functions together with various fundamental properties resulting from the basic definitions. Before we proceed, it is necessary to introduce the notion of the polynomial of degree s over the space R^n.

Definition 3.1: A polynomial of degreee s, is a function of the form

$$P_s(x) = \sum_{i=1}^{\beta(s)} a_i\, y_i(x) \tag{5}$$

where, $x=(x_1,x_2,\ldots,x_n)\epsilon R^n$, a_i are coefficients, $\beta(s)=\binom{n+s}{s}$, and

$$y_i(x) = x_1^{\rho_1} x_2^{\rho_2} \cdots x_n^{\rho_n} \tag{6}$$

where ρ_i are non-negative integers such that $\sum_{i=1}^{n} \rho_i \leq s$.

Example 3.1: In R^2, for s = 2, equ(5) gives

$$p_2(x)=p_2(x_1,x_2) = \sum_{i=1}^{6} a_i\, x_1^{\rho_1}\, x_2^{\rho_2}, \text{ with } \rho_1+\rho_2\leq 2, \text{ or } p_2(x_1,x_2)$$
$$=a_1+a_2x_1+a_3x_2+a_4x_1x_2+a_5x_1^2+a_6x_2^2 .$$

Definition 3.2: The quantity $\phi(f)$ will be called an incremental function of order s, if it results from a spatial function f(x) by a linear operation of the form

$$\phi[f(z)] = \int f(x+z)\ Q(dx) \tag{7}$$

where the measure Q(dx) vanishes outside a bounded support and is such that for every polynomial $p_s(x)$ of degree s

$$Q[f(x)+p_s(x)] = Q[f(x)] \tag{8a}$$

or, due to the linearity of Q,

$$Q[p_s(x)] = 0 \tag{8b}$$

In the following, instead of $\phi[f(z)]$ we will simply write $\phi(f)$ (note that $\phi(f)$ is an incremental function when z=0, as well).

The Q(dx) of equ(7) will be called a measure of order s, belonging to the vector space Ξ of real measures in R^n with finite supports and satisfying equ(8b).

Furthermore, if equ(5) is inserted into equ(8b), we get

$$\sum_{i=1}^{\beta(s)} a_i Q[y_i(x)] = 0 \qquad \text{for all } a_i \tag{9}$$

or

$$Q[y_i(x)] = 0 \qquad i=1,2,\dots,\beta(s) \tag{10}$$

which is equivalent to equ(8b) above. In other words, the measure Q filters out the polynomials up to degree s inherent in the nonstationary function f(x), and leads to a new function $\phi(f)$. In this sense, the relation between f and ϕ is similar to that between a function and its derivative of some order, and so, studying a nonstationary phenomenon using the corresponding incremental function is like studying a surface from its derivatives (of course, such a correspondence may introduce indeterminacy analogous to the one caused by the constant of the integration operation; this will be considered again later).

Example 3.2: Let f(x) be a differentiable function and assume that all its partial derivatives of order s+1 filter out polynomials up to degree s. Then, if we define Q in equ(8b) as the operation of differentiation, the corresponding $\phi(f)$ will be an incremental function of order s (note that the order of differentiation is one higher than that of the incremental function and this is due to the Def.3.2 where s corresponds to the degree of the polyomial $p_s(x)$ filtered).

The discrete versions of the measure Q and the incremental function ϕ , which are useful for the practical applications, may be defined as follows, respectively

$$Q_D = \sum_i q_i \, \delta(x_i) \tag{11}$$

and

$$\phi(x) = \sum_i q_i \, f(x+x_i) \tag{12}$$

where $q_i \in R$, $\delta(x_i)$ is the dirac measure at point $x_i \in R^n$ and, of course, Q_D satisfies equ(8b). The latter is also valid for any element of the vector space Ξ_D, the discrete version of the space Ξ of Def. 3.2. This suggests that the integral of equ(7) is a finite linear expression of the discrete form (12). Under these circumstances, there is no difficulty to prove the following corollary.

Corollary 3.1: For the discrete case defined above equs (11), (12), condition (8b) may be written as

$$\sum_i q_i \, p_s(x_i) = 0 \tag{13}$$

for any polynomial $p_s(x_i)$.

Example 3.3: Consider again the Ex. 3.1 and take the incremental function (12) with $i \leq 5$, $q_{i \leq 4}=1$ and $q_5=-4$ on a square grid, i.e.

$$\begin{aligned}\phi(x) = \phi(\chi_1,\chi_2) &= f(\chi_1+ \Delta\chi,\chi_2) + f(\chi_1,\chi_2+\Delta\chi) + f(\chi_1-\Delta\chi,\chi_2) \\ &+ f(\chi_1,\chi_2-\Delta\chi) -4f(\chi_1,\chi_2)\end{aligned}$$

Then $\phi(\chi_1,\chi_2)$ is an incremental function of order one, as it is easily shown using equs(12) and (13).

Proposition 3.1: The discrete measure Q_D is closed under addition, scalar multiplication and translation.

Proof: The first two properties are trivial consequences of equ(11). The closedness under translation is a direct result of the fact that the polynomials are themselves closed under translation.

Proposition 3.2: If $\hat{f}(x) = \sum_i \xi_i \ f(x_i)$ is the linear estimator of the spatial function f(x) such that

$$\langle f(x)\rangle = \sum_{\ell=o}^{s} a_\ell \ p_\ell(x) \tag{14a}$$

$$\langle \hat{f}(x) - f(x)\rangle = 0 \tag{14b}$$

then the difference $\hat{f}(x)-f(x)$ is an incremental function of order s.

Proof: Using equs(14a), (14b) we find

$$\sum_i \xi_i \langle f(x_i)\rangle - \langle f(x)\rangle = 0 \text{ or}$$

$$\sum_i \xi_i \left\{ \sum_{\ell=o}^{s} a_\ell p_\ell(x_i) \right\} - \sum_{\ell=o}^{s} a_\ell \ p_\ell(x) = 0 \text{ or}$$

$\sum_j \xi_j \ p_\ell(x_j) = 0$, where $x_j = \{x_i, x\}$ and $\ell = 1,2,\ldots,s$. Hence, the $\hat{f}(x)-f(x)$ is incremental of order s.

Remark 3.1: The polynomials defined by equ(5) are useful for determining incremental functions, because they satisfy important geometrical invariance requirements. However, the same role may be played by wider classes of functions, like

$$g(x) = p(x) \exp \sum_i \ b_i \ x_i \tag{15}$$

where $p(x)$ is a polynomial in x and b_i are coefficients (real or complex).

4. Inherent functions of order s

The concept of inherent functions of order s is a natural consequence of that of incremental functions of the same order, and leads to the determinaton of a class of spatial functions with considerable interest regarding functional optimization of nonstationary functions.

Definition 4.1: A spatial function $f(x)$ will be called an inherent spatial function of order s, if the corresponding incremental function $\phi(f)$ is such that

(i) its mean value is

$$\langle\phi(f)\rangle = 0 \tag{16}$$

(ii)there exists a continuous and symmetric function

$$\sigma(h{=}x-x'),\ x,x',h \in R^n, \text{ such that}$$
$$\langle\phi(f)^2\rangle = \int \sigma(x-x')\ Q(dx)\ Q(dx') \tag{17}$$

where $Q \in \Xi$.

The quantity $\sigma(h)$ will be called the inherent covariance of order s, associated to the inherent function $f(x)$ of the same order. Then, $f(x)$ $[\sigma(h)]$ will be said to belong to the class Π[resp.B] of all inherent functions [resp. inherent covariances] of order s.

When inherentity holds true for a spatial function, the corresponding incremental function is by definition stationary and, therefore, if substitute f by ϕ, the limit of equ(2) exists and is finite. Mathematically, the study of the f is now undertaken via the measure Q associated to ϕ, where the latter function has a correlation structure represented via the norms (16) and (17) above. Alternatively, the inherent function may be viewed as a generalized function (as defined by Gelfand and Vilenkin [10]). This is an interesting view which allows some important results of the latter to be used when identifiying the correlation structure of the former, (eg, see latter, Proposition 4.2). Moreover, the Def. 4.1 has its dual meaning within the context of random fields with stationary increments in the sense of Yaglom [11], or that of intrinsic random functions (Matheron [12]).

Remark 4.1: By definition, if $f_1(x)$ as an inherent function of order s, the function

$$f_2(x) = f_1(x) + \sum_{i=0}^{s} a_i x^i \tag{18}$$

where $a_i \in R$, is also inherent of the same order. Therefore, on the basis of equ(18) the two inherent functions $f_1(x)$ and $f_2(x)$ are undistinguishable. In fact, all the problems that may arise using incremental functions are due to the nonexistence of a one to one correspondence between f and ϕ. If we write equ(18) in terms of the corresponding incremental functions we find

$$\phi_2(x) = \phi_1(x) \tag{19}$$

i.e. any ϕ_2 derived from f_2 using a measure Q such as in Def. 4.1, equals the incremental function ϕ_1 derived from f_1 using the same Q (of course, the converse is not valid). Fortunately, for the optimization methodology presented in this paper, the representation (18) does not cause any problem of indeterminacy.

The following proposition establishes an interesting link between the correlation structure of the initial, inherent function and that of the corresponding incremental function.

Proposition 4.1 If f(x) is an inherent function of order s, then

$$\langle f(x),\ f(x')\rangle = \sigma(h=x-x') + P(x,x') \tag{20}$$

where P(x,x') is a polynomial in x,x' representing the nonstationary features of the norm $\langle f(x),f(x')\rangle$.

Proof: According to Prop. 3.2, the function

$\phi(x) = f(x) - \sum_{i=o}^{s} b_i\, x^i$ is incremental of order s for proper coefficients

b_i. Then, taking the norms of the last equation assuming that

$Q(x) = \delta(x) - \sum_i q_i\, x^i$, we derive equ(20).

It is noteworthy that, while equ(20) is theoretically remarkable, it is usually not applicable in practice since the nonstationary part P(x,x') may be in general not computable from the data available. Fortunately, as we will see in the next section, within the context of functional optimization it is only the stationary part σ(h) that interests us.

Example 4.1: Let $f(x) = p_s(x) + w(x)$, where $w(x)$ is a zero mean stationary function with an ordinary covariance $c(h)$. Then, the $f(x)$ is an inherent function of order s with $\sigma(h) = c(h)$.

Remark 4.2: The class Π of all inherent functions of order s is larger than that of all functions resulting from the superposition of a polynomial of degree s on a zero mean stationary function. This is intuitively clear, since the only link between the inherent model and the reality is through the incremental functions. Obviously, the same is valid for the corresponding covariances (eg, in R^1 and s=0, the function $\sigma(h) = -h$ can be used as an inherent but not as an ordinary covariance).

Clearly, not every function can play the role of an inherent covariance $\sigma(h)$, as specified by Def.4.1. It has to be such that the norm (17) is non-negative. Relevant to this requirement is the following definition.

Definition 4.2: A continuous and symmetric function $\sigma(h)$, $h \in R^n$, is said to be conditionally positive definite of order s and thus a valid inherent covariance model of the same order, if and only if

$$\langle \phi(f)^2 \rangle = \int \sigma(h=x-x') \; Q(dx) \; Q(dx') \geq 0 \qquad (21)$$

for all measures $Q \in \Xi$ of order s. The discrete version of equ(21), useful for practical applications, has as follows

$$\langle \phi(f)^2 \rangle = \sum_{i,j} q_i \; q_j \; \sigma(h=x-x') \geq 0 \qquad (22)$$

for all $q_i, q_j \in \Xi_D$.

The converse is also true, i.e., to any valid $\sigma(h)$ of order s corresponds an inherent function f(x) of the same order.

Example 4.2: In R^1 and s=0, equ(22) gives $\langle\phi(f)^2\rangle = -2\sigma(x-x') \geq 0$.

The proposition below offers a representation of the inherent covariance $\sigma(h)$, in the frequency domain.

Proposition 4.2: A continuous and symmetric function $h \in R^n$, is an inherent covariance of order s, if and only if it can be represented as

$$\sigma(h) = \int_{R^n} [\cos\,(wh) - T_s(wh)]\ \frac{\Lambda(dw)}{|w|^{2s+2}} + P(h) \tag{23}$$

where, $w = (\omega_1, \omega_2, \ldots, \omega_n) \in R^n$ are frequency coordinates,

$T_s(wh) = \sum_{p=o}^{s} (-1)^P (wh)^{2p}/2p!$, P(h) is a polynomial of degree not greater than 2s, and $\Lambda(dw)$ is a positive symmetric measure including no dirac-functions $\delta(w)$ and such that

$$\int_{R^n} \Lambda(dw)\ /\ (1 + w^2)^{s+1} < \infty \tag{24}$$

Proof: Since we may define the inherent function as a generalized one of order s, see discussion following Def.4.1, the proof is a straightforward application of the theory of generalized functions (Gelfand and Vilenkin [10], Chapter II).

Corollary 4.1.: In the isotropic case, where

$$\sigma(h) = \sigma(r=|h|) \tag{25}$$

the expression (23) may be rewritten in terms of polar coordinates as

$$\sigma(r) = \int_0^\infty [\Theta_n(\omega r) - T_s(\omega r)]\, dF(\omega) + P(r) \tag{26}$$

where, $\omega=|w|$, $\Theta_n(\omega r)= G(\frac{n}{2})\ [\frac{2}{\omega r}]^{(n-2)/2}\ J_{\frac{n-2}{2}}(\omega r)$, G is the gamma function, J_m is the Bessel function of first kind and order m (Gradshteyn and Ryzhik [11]) and F(w) is a non-decreasing function on R_+, derived from the measure Λ(dw) of equ(23) when we go over polar coordinates.

Another useful result concerning the characterization of the inherent covariance in the isotropic case, is given below (Christakos [9],[12]).

Corollary 4.2: A continuous and symmetric function $\sigma(r)$, is an isotropic inherent covariance of order s, if and only if

(i) it is valid

$$\lim \frac{\sigma(r)}{r^{2s+2}} = 0 \quad \text{when } r\to\infty \tag{27}$$

and

(ii) its spectral function (Hankel transform) $S_n(\omega)$, exists in the sense of generalized functions, does not contain any dirac-functions $\delta(\omega)$, and is such that

$$\omega^{2s+2} S_n(\omega) \geq 0 \tag{28}$$

Remark 4.1: Within the framework of space transformations as reported in [13], the spectral functions $S_n(\omega)$ of an inherent covariance $\sigma(r)$ on spaces of various dimensionalities, belong to the family of functions for which the relationships below are valid

$$S_{n+1}(\omega) = -\frac{1}{\pi} \int_{\omega}^{\infty} \frac{dS_n(v)}{dv} (v^2-\omega^2)^{-1/2} dv \tag{29}$$

$$S_{n+2}(\omega) = -\frac{1}{2\pi\omega} \frac{dS_n(\omega)}{d\omega} \tag{30}$$

The inverse and other relevant expressions may be found in the same reference.

Corollary 4.2, together with equs (29), (30), may serve as an analytically and computationally tractable criterion to test whether a particular function omay be used as an inherent covariance. For example, if employ covariances of the polynomial form

$$\sigma(r) = \sum_{\ell=0}^{m} (-1)^{\ell+1} c_\ell \, r^{2\ell+1} + a\,\delta(r) \tag{31}$$

the Corollary 4.2 leads to the following constraints regarding equ(31)

$$m=s, \qquad a \geq 0 \qquad \text{and}$$

$$\sum_{\ell=0}^{s} (2\ell+1)! \frac{\pi \, c_\ell}{\ell! \; G(\frac{n}{2})} G(\ell + \frac{n+1}{2}) \, \omega^{s-\ell} \geq 0 \tag{32}$$

Example 4.3: If $s = 2$, equ(32) gives in R^n,

$$a,\ c_o\ c_2 > 0 \qquad \text{and } c_1 > -2\sqrt{\frac{5}{3}\frac{n+3}{n+1} c_o\ c_2} \tag{33}$$

5. The solution of the Problem P_o

As was mentioned in section 2, the solution of the problem P_o coincides with the determination of the values of the coefficients ξ_i that satisfy assertions (4c) and (4d). The idea is to obtain the ξ_i by means of incremental functions, since according to the foregoing theory the latter are the ones to have computable norms and, thus, make Problem P_o well defined. Doing so, the following lemma is the link between the theory of inherent functions and the Problem P_o.

Lemma 5.1: For the case of inherent spatial functions $f(x)$ of order s, the equations (4c), (4d) may be written as

$$\langle\{\hat{\Psi}[f\} - \Psi[f]\}^2\rangle = \sum_{i,j} \xi_i\ \xi_j\ \sigma(x_i - x\ ) - 2\sum_i \xi_i \int \sigma(x-x_i)\ \Psi(dx) + \int \sigma(x-x')\ \Psi(dx)\ \Psi(dx') = \text{minimum} \tag{34}$$

and

$$\sum_i \xi_i\ y_\ell(x_i) = \Psi[y_\ell(x)] \tag{35}$$

where $x_i, x_j \in S$ (S is a subset of data points), $\ell = 1,2,\ldots, \beta(s)$ and the measure $\Psi(dx)$ is defined as above (see discussion following equ(3b)).

Proof: From the theory developed in the preceding sections it is obvious that equ(4d) holds for an inherent function f(x) of order s, if the difference $\hat{\Psi}[f] - \Psi[f]$ is an incremental function also of order s, i.e.

$$\hat{\Psi}\,[y_\ell] = \Psi[y_\ell] \tag{36}$$

$\ell=1,2,\ldots,\beta(s)$, and then equ(35) follows without any difficulty. Lastly, using dqu(17) for the above incremental function together with the equ(4c), the latter leads after some algebraic manipulations to equ(34).

It is interesting to point out that while we estimate the nonstationary function f(x), we only need the stationary part $\sigma(h)$ of its correlation structure, see equ(20) above.

Now we are ready to finally give Problem P_o the well-defined form, below.

Problem P_F: Find the optimal estimator $\hat{\Psi}[f]$ of the linear functional $\Psi[f]$ of equ(1), so that the conditions (4a), (4b), (34) and (35), are satisfied, where f is an inherent function of order s and $\sigma(.)$ is the corresponding inherent covariance.

The solution of Problem P_o is introduced by the following proposition

Proposition 5.1: The Problem P_F is perfectly solved if we determine the coefficients ξ_i that satisfy the set of equations

$$\sum_i \xi_i\, \sigma(x_i - x_j) + \sum_\ell \nu_\ell\, y_\ell\,(x_j) = \int \sigma(x - x_j)\, \Psi(dx) \tag{37}$$

and

$$\sum_i \xi_i\, y_\ell\,(x_i) = \int y_\ell(x)\, \Psi(dx) \tag{38}$$

where x_i, $x_j \in S$, ν_ℓ are Lagrange multipliers and $\ell=1,2,\ldots,\beta(s)$

<u>Proof:</u> Starting from equs(34), (35), and after introducing the Lagrange multipliers ν_ℓ, we seek the minimization of the quantity

$$\langle\{\hat{\Psi}[f] - \Psi[f]\}^2\rangle + \sum_\ell \nu_\ell \left\{\sum_i \xi_i \, y_\ell \, (x_i) - \Psi[y_\ell]\right\} \tag{39}$$

with respect to ξ_i and ν_ℓ. Taking derivatives of equ(39) with respect to ξ_i, ν_ℓ, and setting them equal to zero, we obtain after some algebraic manipulations the equs(37), (38).

The solution of the Problem P_F is completed as soon as we substitute the values of the coefficients ξ_i into equs (4a) and (34) to obtain the functional estimator and its accuracy (or estimation error), respectively. Alternative expressions for the accuracy (34) may be found in [9].

Here we should point out similarities of the solution obtained above with that derived in terms of the classical stochastic theory (time series, Wiener [1]; intrinsic kriging, Matheron [3]). Apparently, despite the fact that the non-stochastic and the stochastic models are conceptually completely different, they may lead to several similar results. However one cannot always derive conclusions regarding non-stochastic spatial data from results on stochastic functions. For example, no prediction theory for general individual time series can be deduced directly from the prediction theory of random processes (Masani, [14])

<u>Remark 5.1:</u> The system of equs(37), (38) will have a unique solution if and only if the basic functions $y_\ell(x_i)$ are independent of the data points. Consequently, if two of the measurements are made at the same point, the

system will have not a solution, because two rows of the covariance matrix will be identical. It can also be shown that the set of equs(37), (38) is invariant to the system of coordinates used, [9].

Remark 5.2: From equ(34) we see that the accuracy of the functional estimator is independent of the data values $f(x_i)$. It is instead affected by the relative geometries of the data points and the functional support F (equ(1)), and also the spatial structure of the function f(x) as it is expressed through the inherent covariance model $\sigma(h)$. Therefore, once these features are known, the corresponding accuracy can be calculated before any measurements are made.

Remark 5.3: In the case of point functional, see equ(3a), we substitute the right parts of equs(37), (38) with $\sigma(x-x_j)$ and $y_\ell(x)$, respectively. Then, if x coincides with a data point x_i, the solution of the above equations give $\xi_i=1$ and $\xi_j=0$, $i\neq j$. This immediately implies

$$\hat{\Psi}[f] = \hat{f}(x_i) = f(x_i) \quad \text{and} \quad \langle\{\hat{\Psi}[f] - \Psi\,[f]\}^2\rangle =$$

$$\langle\{\hat{f}(x_i) - f(x_i)\}^2\rangle = 0 \;,$$

i.e. the estimation methodology proposed is a perfect interpolator (when there is not measurement error it restores the measured values at the data points). Such estimators are, certainly, very desirable. Lastly, note that the system of equs(37), (38) may be adapted to the case of measurements including errors by adding to the covariance terms the proper norms of measurement errors.

6. Procedure and application

The foregoing theoretical results may lead to general computational procedures regarding solution of the Problem P_F on a computer. Apparently, the practical problems encountered are mainly related to the determination of the order s and the covariance $\sigma(r)$. One, possible, computational procedure is outlined below, and is based on an approximate but simple parameter estimation approach (of which a detailed description may be found in [9]).

Step 1: Identify the order s of inherentity based on the available data values. One way to do this in practice is to estimate some known points from neighboring data values, assuming a covariance $\sigma(r)$ and setting in turn $s=0,1,2$. The s value that gives the smallest, on average, estimation error will be chosen as the order of inherentity in the spatial variation.

Step 2: Assume that the inherent covariance $\sigma(h)$ is of the polynomial type, see equ(31), and determine the coefficients a, c_ℓ, for all covariances that are appropriate for the above order s (i.e. polynomials of degree $< 2s+1$) and also satisfy the constraints of equ(32). Usually, some incremental functions of order s are generated from the data assuming a combination $\{s,\sigma(r)\}$, and then we require the minimization of the sum of the squared differences between them and the theoretical incremental functions expressed in terms of the coefficients a, c_ℓ.

Step 3: Select among all the covariances defined in Step 2, the one that best describes the spatial variation. This is done by estimating a number of data points for each one of the combinations $\{s,\sigma(r)\}$ defined above, and evaluating the average estimation error. The best inherent covariance is the one that gives the lowest on average error.

Steps 1, 2, and 3 constitute the structure identification part of the procedure, regarding the spatial variation of the studied function.

Step 4: Solve the system of equa(37), (38) with respect to the coefficients ξ_i and ν_ℓ . At this point, the symmetry of the data configurations may be very helpful in reducing the computational effort.

Step 5: Substitute the above coefficients into equs(4a) and (34) to obtain the functional estimator and its accuracy (or estimation error) respectively.

Remark 6.1: It is noteworthy that the above procedure leads to a solution of the optimization problem which relies on the stationarity of the incremental functions of order s. The trend is automatically cancelled by taking increments of order s and, therefore, it does not need to be estimated and subtracted from the data (as in other popular methods, see eg, [15]). Instead, it is identified solely on the basis of the order s of inherentity (which corresponds to the degree of the polynomial filtered).

An application is discussed aiming at the illustration at the above procedure: The spatial function selected is the water table elevation (in feet) in an area that includes most of the Equus Beds, a major aquifer in Kansas. The Equus Beds produce groundwater through more then 2,000 industrial, municipal and irrigation wells in several counties in the south-central part of the State of Kansas. Data used in this study were the January 1981 ones, which are available at the points depicted in Fig. 1. Starting with the structure identification of the data pattern, the procedure will first determine the order s of inherentity using neighborhoods of about sixteen data points. We find that the order s=1 gives the smallest on average error (step 1) and, therefore, the spatial variability may be characterized by the existence of a linear trend. The latter, however, is not estimated but only identified by its degree s=1. For this degree, three polynomial covariance models of the type (31) may be fitted: $\sigma(r)=28.75$, $\sigma(r)= -24.22r$ and $\sigma(r)=2.33\ r^3$. These three models are appropriate for s=1 and satisfy constraints (32), see step 2. Among them, the second one best describes the spatial variability since it gives the lowest on average error, in estimating the data points (step 3). Next, we seek the optimal estimation of the point functional $\Psi[f] = f(x)$, see equ(3a) and Rem. 5.3. Using the information found above at the structure identification part of the procedure, we proceed to the second part which solves the corresponding system of equations (steps 4 and 5) to obtain values for the water table elevation and their accuracies, at numerous points on a properly specified grid. These values are then used as input to a plotting program to produce the contour maps of the estimated water table elevation (in feet, Fig. 1) and the associated estimation errors (in feet^2, Fig. 2). The corresponding block diagrams which offer another view of the morphology of the estimation and error variance surfaces are shown in Figs. 3 and 4 respectively. Due to the relative small number of data at some parts of the pattern, one should expect rather large errors there. Certainly, if the number of data points increase the accuracy will be improved. Indeed, if one takes advantage of the aforementioned property of the estimation procedure (i.e., the estimation error does not depend on the data values but only on the spatial variation and the locations of the data points, see Rem. 5.2), and compute the estimation errors for, say, five more data points at the NE part of the pattern, the accuracy will be improved in this area by about seven per cent.

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Figure Legends

Figure 1: Contour map of estimated water table elevation in the Equus Beds. Locations of observation wells are also shown.

Figure 2: Contour map of the error variance associated to map of Fig.1. Locations of observation wells are also shown.

Figure 3: Block diagram of the estimated surface.

Figure 4: Block diagram of the error variance surface.

EQUUS DATA SET: ESTIMATES
PLOT NO. 1 DATE 09/22/86 TIME 16:12:23

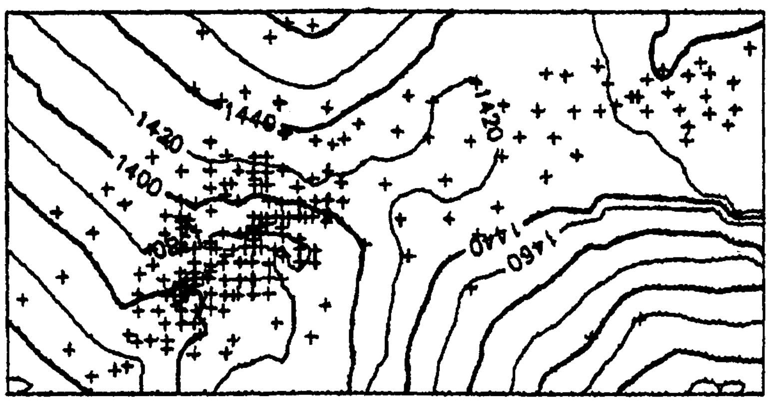

Figure 1

EQUUS DATA SET: ERROR IN ESTIMATES
PLOT NO. 1 DATE 09/22/86 TIME 16:13:57

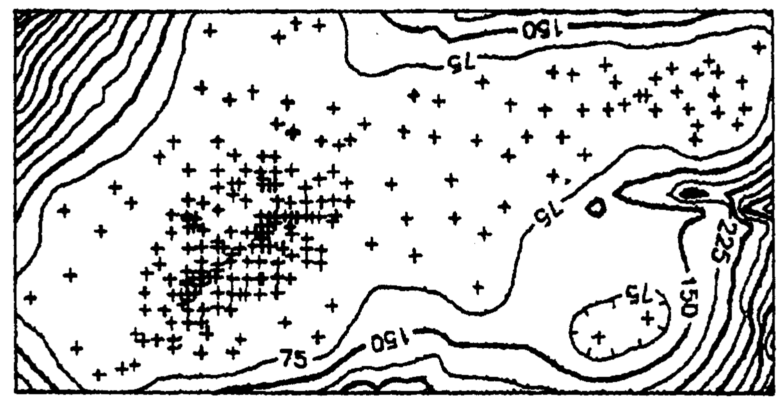

Figure 2

Figure 3

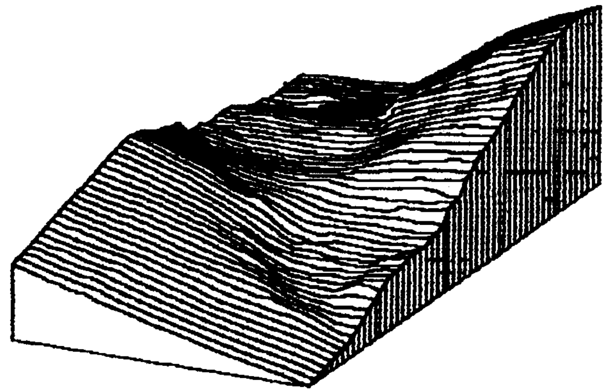

Figure 4