INTERPOLATION WITH POSITIVE DEFINITE FUNCTIONS

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CONTENTS

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ABSTRACT

It is well-known that kriging and interpolation by splines are equivalent. Kriging is based on a stochastic formulation whereas splines are formulated in a deterministic way. A third presentation is given in terms of Radial Basis Functions. The connections between these three are described in elementary terms and implications for the properties of the kriging estimator are reviewed as they relate to interpolation by Radial Basis Functions. Results given by Micchelli are used to obtain new models for generalized covariances.

RESUME

Il est bien connu krigeage et spline plaque mince sont presque la même chose. Le krigeage est basé sur un modèle de fonctions aléatoires intrinseques alors que les splines sont déterministes. Une troisième présentation du problème est donnée par ce qui s'appelle en anglais "Radial Basis Functions". Avec ces nouvelles idées, il est facile d'expliquer les rapports entre les trois. Mais on peut dire que celle de l'estimateur de krigeage demeure la plus générale. Par conséquent, il est plus commode d'expliquer les caractéristiques du krigeage que les autres. Les résultats de Micchelli nous donnent de nouveaux modèles pour les covariances généralisées.

A - INTRODUCTION

One of the distinguishing features of geostatistics is the use of the variogram (or more generally the generalized covariance) in place of the covariance even though the kriging estimator is obtained by minimizing the estimation variance. In particular the use of the variogram precludes the necesity of knowing a constant drift and the use of the generalized covariance only requires knowing the order of the drift. Both the variogram and generalized covariances must satisfy a generalized positivity condition as well as a growth condition. From the perspective of a stochastic formulation the positivity condition is necessary to ensure that the estimation variance is non-negative and hence that the minimized value is non-negative.

An important characteristic of the kriging estimator is that the weights, i.e., the kriging equations do not depend on the data but rather only on the variogram (or covariance funtion) and on the sample pattern. This characteristic suggests that the estimation process is not as truly stochastic as its derivation would make it appear. It has been known for some time, although not recognized in all of the literature, that kriging and thin plate splines are essentially the same. Both the form of the spline as well as the coefficents are obtained by an optimization step where as for the kriging estimator it is the kriging system (i.e.,the weights in the estimator) that is obtained by optimization. In one part of the.the literature the problem is posed as simply one of interpolation and of sufficient conditions for the eixtence/uniqueness of the interpolator. While kriging, i.e., the estimation process that is at the heart of geostatistics, is not thought of as primarily an interpolator one finds that these various approaches are linked by the key concept of positive definiteness. An examination of this concept and how it relates to the various approaches provides additional insight into the relationship between these different methods.

B - POSITIVE DEFINITENESS

1 - A REVIEW

The usual way to define positive definiteness for complex valued functions defined on n-dimensional Euclidean space is the following:

G(x) is positive definite if

$$\sum\sum \lambda_i \bar{\lambda}_j G(x_i - x_j) \geq 0 \quad \text{for all complex numbers } \lambda_1, \ldots, \lambda_n \text{ and all points } x_1, \ldots, x_n \qquad (1)$$

As noted by Stewart (1976) interest in positive definite functions of a real variable dates from at least 1923 in the work of Mathias but was in fact preceded by the work on positive definite kernels by Mercer in 1909 who was interested in the solution of certain integral equations. The connection with interpolation appeared early in the work of E. H. Moore in 1919 who defined positive definite kernels by the reproducing property, this formulation is very nearly the same as that of the dual form of simple kriging.

When fitting variograms it is not uncommon to fit a model to only a part of the sample variogram. This aproach is related to the question of determining the existence of a positive definite function on all of Euclidean space given one that is positive definite only in a neighborhood of the origin. For example, in one dimension consider the interval (-a,a), in this case the extension problem was solved by Krein in 1940 but in higher dimensions the existence of an extension depends in a critical way on the shape of the neighborhood.

In probability and statistics (and geostatistics) positive definite functions are important because they are covariances or alternatively because they are the Fourier transforms of probability distributions. In turn positive definite functions are intimately connected with positive definite matrices. This connection is very imortant for continuous functions and will be pursued further in the next section. Positive definite matrices have all kinds of nice properties, for example they have square roots or they can be used to define a metric and all the eigenvalues are positive. Multivariate techniques such as factor analysis, principal components analysis and correspondance analysis all depend on the properties of positive definite matrices, in particular the diagonalizability property. The definition given above in (1) is essentially that of a positive definite matrix.

2 - GENERALIZATIONS

It was noticed by early workers in the field that one might replace the finite sum condition given in (1) by an integral instead, as in the following:

$$\iint G(x-y)\Phi(x)\Phi(y)dxdy \geqslant 0 \qquad (2)$$

with the Φ in some suitable collection of functions. One must of course make some assumptions about the integrability of G and Φ to ensure the existence of the integral in (2). If G is continuous and the Φ are in the collection of continuous functions that vanish outside of a compact set then (1) and (2) are equivalent. However if the continuity restriction on G is deleted then there are unbounded functions that satisfy (2) and hence they are not (ordinary) covariances. Stewart (1976) provides a quick overview of the work of Cooper in characterizing functions that satisfy (2) for Φ in various spaces of functions. The variogram and generalized covariances arise not from using (2) in lieu of (1) but rather in following the idea suggested by the use of (2) namely the weight vectors $[\lambda_1,\ldots,\lambda_n]$ which are analogous to the functions Φ must satisfy some auxillary condition(s). In the light of Cooper's results it is not surprising that variograms in particular need not be bounded. Matheron(1973) (and elsewhere in earlier work) generalized the condition in (1) by imposing conditions on the weight vectors to ensure that the variance of authorized linear combinations could be computed as though the random function had a true covariance.

In geostatistics and in the context of interpolation integrability as in (2) is not a problem since only finite sums are of concern. Likewise the conditions to be imposed on the weight vector are not quite in the nature of a growth condition but are certainly analogous. In the development of the theory of intrinsic random functions polynomials play a central role since they are translation invariant and this was necessary to obtain the stationarity of the authorized linear combination and this results in the familiar universality conditions. As will be seen later in the context of interpolation from a deterministic perspective it is the linear independence of the polynomials that is important. A general formulation might be as follows:

Definition 1

Let G(x) be defined (and real valued) at each point of a subset A of Euclidean m-space. Let $K=\{k_0(x),\ldots,k_p(x)\}$ be a collection of functions defined at each point of A and linearly independent on A. Then G is said to be positive definite on A with respect to the class K if

$$\sum\sum\lambda_i\lambda_j G(x_i-x_j) \geq 0 \tag{3}$$

for all points $x_1,\ldots,x_n$ in A and for all weight vectors $[\lambda_1,\ldots,\lambda_n]$ satisfying

$$\sum\lambda_i k_j(x_i) = 0 \;;\; j=0,\ldots,p \tag{4}$$

Note that symmetry is a consequence of (3). Of course if K were $\Pi_{r-1}(R^m)$ the space of polynomials in m variables, of degree less than or equal to r-1, A were Euclidean m-space and G were assumed continuous then this would be the definition of conditionally positive definite as given in Matheron(1973). Two other observations are in order, first there is no explicit condition on the growth of G (continuous variograms are dominated by a quadratic) and secondly as in the special case given by Matheron such functions would be unique only upto a term for which (3) is identically zero.

We digress briefly to give an important special case, in the following A is Euclidean m-space and K consists only of the one function which is identically 1. G is said to be conditionally positive definite (order zero) if

$$\sum\sum\xi_i\xi_j[G(x_i-x_j)-G(x_i)-G(x_j)]\geq 0 \tag{3'}$$

for all $x_1,\ldots,x_n$ in A and all weight vectors $[\xi_1,\ldots,\xi_n]$. As was shown by Johansen(1966) this condition is equivalent to (3) with the specified A and K. The latter is of course the familiar condition for (the negative of) a variogram.

Note that if A is taken to be a finite set,for example the set of sample locations, then the class of postive definite functions is much larger. This is essentially the idea put forward by Dunn (1983) although not in the guise of a new definition. In particular for a regular grid the sample variogram will satisfy the positive definiteness condition. As noted in Myers (1984) (and reply by Dunn (1984)) this is not sufficient for kriging in any practical sense. Without the use of a valid theoretical model one would still be unable to evaluate the terms on the right hand side of the kriging equations. In order to see whether this more general definition of positive definiteness is of any practical use it will be useful to recall some known results about representation theorems and tests for positive definiteness as well as to examine the class of positive definite functions under the various choices of K.

3 - REPRESENTATION THEOREMS AND SUFFICIENT CONDITIONS

Although this paper is not primarily concerned with either of these topics it is useful to review known (and perhaps not so well-known) results, for a more complete discussion an excellent summary is found in Stewart (1976). The best-known representation theorem is the form given by Bochner, that is, continuous positive definite functions vanishing at the origin are Fourier Transforms. A version of this theorem was given by Mathias (see Stewart (1976)) and it has been extended to more general contexts such as locally compact Abelian groups and operator algebras. Stewart has given such an extension for the generalization of positive definiteness given by Cooper. Matheron (1973) obtained a representation therorem for generalized covariances which incorporates the Bochner theorem as a special case. All of these representations are given in integral form, hence to determine whether a particular function is positive definite would in general require solving an integral equation or inverting a Fourier transform. The condition given in (1) (or more generally as in (3)) is difficult to verify in practice since the condition must be satisfied for all points in A and all weight vectors satisfying the auxillary conditions. In practice each function must be tested by a method or approach that is special for that function, this is aptly illustrated in Armstrong and Diamond(1984)

We note three results that are of practical use in testing for positive definiteness (in addition to those demonstrated by Armstrong and Diamond).The first is not a representation theorem in the sense indicated above whereas the second is a consequence of the general Bochner representation theorem. The third provides for easy construction of positive definite functions.

a. It was shown by Johansen (1966) that Conditional positive definiteness of G (see equation (3') above) is equivalent to the positive definiteness of $\exp(\alpha F)$ ($\alpha > 0$) in the sense of (1). This means that variograms can be obtained as the logarithms of covariances. One note of caution, $G(t)=t^2$ is conditionally positive definite on the real line but does not satisfy the growth condition for a variogram. More generally this relationship relates conditionally positive definite functions to the logarithms of infinitely divisible characteristic functions.

b. The second result is given by Micchelli(1986) and its presentation requires additional notation and terminology;

G(t) defined on $(0,\infty)$ is completely monotonic if G is infinitely differentiable and if $(-1)^l G^{(l)}(t) > 0$ for $l=1,2,\ldots$ and all t.

Let $\mathcal{P}_K(R^m)$ be the class of positive definite functions (satisfying condition (3),(4)) where A is Euclidean m-space and K is $\Pi_{r-1}(R^m)$. $\mathcal{P}_K$ the intersection of these classes for m=1,....

Theorem (Micchelli)

F is in $\mathcal{P}_K$ if $G(t)=F(\sqrt{t})$ is continuous on $[0,\infty)$ and $(-1)^r G^{(r)}$ is completely monotonic on $(0,\infty)$.

The proof of this theorem uses a result due to Bernstein on the representation of completely monotonic functions as Laplace transforms.
Micchelli gives several other extensions of this theorem but we will simply give some examples of its application.

c. The third result is found in Powell (1985) and is easily proven directly. Let F(t) be given by

$$F(t) = \int \exp(-ut^2)\psi(u)du \tag{5}$$

where $\psi(u)$ is a non-negative function such that the integral in (5) is finite and for which there exist $0<a<b$ such that

$$\int \psi(u)du > 0$$

then F is positive definite. Alternatively suppose that F is differentiable and that F' is given by

$$F'(t) = t\int \exp(-ut^2)\psi(u)du \tag{6}$$

and ψ satisfies the same conditions as above then F is conditionally positive definite.

4 - SOME PROPERTIES

The original definition of positive definiteness given by Mathias in 1923 included a symmetry condition, but as was noted by Riesz the symmetry is a consequence of (1). More generally for positive definiteness in the sense of (3) symmetry is a consequence if the function vanishes at the origin. If the constant function is included in K then this restriction imposes no new conditions.

It is well-known that the classes of functions positive definite in the sense of (1) (or more generally in sense of (3)) are closed under positive linear combinations which justifies the use of nested models. The class of functions positive definite in the sense of (1) is also closed under multiplication and with respect to pointwise limits. Moreover if the functions are continuous then pointwise convergence is equivalent to uniform convergence on compact sets (this result is valid even in the context of locally compact Abelian groups). The closure under multiplication does not extend to conditionally positive definite functions (i.e., variograms) and certainly not to generalized covariances. The closure under point-wise limits is easily extended to positive definiteness in the sense of (3) since the function is considered at only a finite number of points at any one time hence it follows directly from the definitions of positive definiteness and point-wise convergence. The latter is of interest in view of the results of Armstrong and Diamond (1984), Myers (1985) and Myers (1986) on the continuity of the kriging estimator with respect to the variogram.

Let $K_2 \supset K_1$ be two sets of linearly independent functions then the class of positive definite functions (in the sense of Definition 1) with respect to K_1 and A is contained in the class positive definite with respect to K_2 and A. Likewise if $A_1 \supset A_2$ are two sets in R^n then the class of functions positive definite with respect to A_1 and K is contained in the class positive definite with respect to A_2 and K.

The class of positive definite functions is also closed with respect to convolution in a certain sense. For the case of conditionally positive definite functions (Eq. 3') the result is given in Johansen but it is easily seen to be valid for Definition 1 as well:

Lemma (Johansen) Let q be real, continuous, symmetric and conditionally positive definite with respect to A and K. Further let T be a finite subset such that u-s+t is in A for all u in A, s and t in T. For any function k defined on T form

$$\Phi(u) = \Sigma\Sigma\ k(s)q(u-s+t)k(t) \tag{7}$$

then Φ is continuous, symmetric and positive definite.

Covariances must be bounded, variograms must grow slower than a quadratic and in general the growth condition is related to the presence or absence of drift (Theorem 2.2, Matheron (1973)). It may not be so obvious that positive definiteness and the growth condition are separate properties but an example easily illustrates this; t^α , $0 < \alpha < 2$ satisfies both the growth condition and produces a conditionally positive definite function. The latter condition is satisfied even for $\alpha = 2$ but the growth condition is violated.

5 - EXAMPLES

In practice variograms are modelled as positive linear combinations of valid models such as the spherical, power, exponential, gaussian, logarithmic and cubic. For generalized covariances the choice is usually limited to polynomial models. It could be useful then to expand the list of such models. As an application of Micchelli's theorem we find that

$$G(t)= 1/[t+c]^\alpha \quad , \ c>0 \text{ and } \alpha>0 \tag{8}$$

is completely monotonic. Furthermore

$$F(t) = (c + t^2)^{r-\alpha}\ ,\ c>0 \text{ and } 0< \alpha < 1 \tag{9}$$

$$F(t) = -(c + t2)^r \log(c + t^2),\ c>0 \tag{10}$$

are in $\mathcal{P}_K$. For the case of c=0, k=1 (10) becomes the familiar "spline term" in generalized covariances. In the case of $\alpha=1/2$, c=1 (9) gives Hardy's multiquadratic function (see Hardy (1971)).

It should be noted that in the case of (8),(9), F(0) is not zero and hence to obtain variograms in the usual sense we must consider F(0)-F(t).

Let q be a spherical variogram with range a and T $=\left[0,\ a/2,\ a\right]$, after applying Johansen's lemma we find that Φ is not spherical, has range 2a and incorporates second degree terms.

C – INTERPOLATION AND DUALITY

1 – DUAL FORM OF KRIGING

If instead of writing the punctual Kriging estimator in the usual form

$$Z^*(x_0) = \Sigma\lambda_i Z(x_i) \tag{11}$$

where the weight vector satisfies the usual Kriging equations

$$\Sigma\lambda_i\gamma(x_i-x_j) + \Sigma\mu_l k_l(x_j) = \gamma(x_0-x_j)$$

$$\Sigma\lambda_i k_l(x_i) = k_l(x_0);\ l=0,\ldots p\ ,\ j=1,\ldots n$$

or in the simpler matrix form

$$\begin{bmatrix} K & F \\ F^T & 0 \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \end{bmatrix} = \begin{bmatrix} K_0 \\ k_0 \end{bmatrix} \tag{12}$$

$Z^*(x_0)$ is written in the dual form

$$Z^*(x_0) = \Sigma b_i\gamma(x_0-x_i) + \Sigma a_l k_l(x_0) \tag{13}$$

then the vectors $a^T = [a_0,\ldots a_p]$, $b^T = [b_1,\ldots b_n]$ are obtained from the system

$$\begin{bmatrix} K & F \\ FT & 0 \end{bmatrix} \begin{bmatrix} b \\ a \end{bmatrix} = \begin{bmatrix} Z \\ 0 \end{bmatrix} \tag{14}$$

The coefficient matrices in (12) and (14) are the same and a unique solution is obtained if that matrix is invertible. It will be seen that invertibility is a consequence of positive definiteness. As is shown in Myers (1986) the general cokriging estimator may be written in dual form in a completely analogous way. In obtaining the system (11) the variance of the error of estimation is minimized and exactness is a (happy) by-product of that optimization. In contrast thin plate splines are obtained by an optimization conditioned on the exactness.

2 - RADIAL BASIS FUNCTIONS

In the context of numerical approximation the following problem has received considerable attention:

Given an unknown function $Z(x)$, x in some region A find an approximating function $Z^*(x)$ which coincides with $Z(x)$ at a finite number of specified locations. The approximating function might be subject to some additional conditions such as differentiability or the minimization of some loss function.

One approach is to assume that the aproximating function is a linear combination of known basis functions and in particular to assume that the approximating function is of the form

$$Z^*(x) = \Sigma b_i g(x,x_i) \tag{15}$$

or more generally

$$Z^*(x) = \Sigma b_i g(x,x_i) + \Sigma a_j k_j(x) \tag{15'}$$

and the functions $g(x,x_i)$ were frequently taken to be of the form $\gamma(d_{xi})$ where d_{xi} is the distance (i.e., radius) between x and x_i and hence the name Radial Basis functions as used in Michelli and in Powell. The functions $k_0,\ldots,k_p$ are usually polynomials. If the exactness condition is imposed, i.e., $Z^*(x_i)= Z(x_i)$, $i=1,\ldots,n$ then the coefficents in (15) are obtained as the solution to a system of linear equations. Hardy (1971) used a particular choice of g and called the interpolated surface Multiquadratic. It was soon noted that for some choices of the Radial Basis function that the coefficent matrix could be singular, at least for some data configurations, and interest arose in finding sufficient conditions to insure the existence. Note that Inverse Distance Weighting is an interpolation process of this kind. It was subsequently proposed that the estimator (15) be replaced by one like (13) (i.e. like (15')) for two reasons; first the polynomial terms would ensure that if $Z(x)$ were a polynomial of that degree or less then the approximation would be an exact fit, secondly it was argued that this would make the coefficient matrix invertible when it might not be otherwise. Micchelli has defined positive definiteness in a manner almost like equation (3) but restricts it to isotropic functions in the context of showing that the positive definiteness is sufficent to ensure the invertibility of the coefficent matrix in (14).

3 - A SUFFICIENT CONDITION

Although the following result is not completely new (it is given in a special form by Micchelli and by Powell, it also apears as consequence of the derivation of the BLUE in Matheron (1973)) the more general form is of interest both because of the result and because of the simplicity of the proof.

Theorem

Let G be positive definite in the sense of (3) then for any choice of $x_1, \ldots, x_n$ in A the coefficent matrix in (14) is invertible and hence G may be used with an estimator/interpolator of the form (13) to interpolate Z.

Suppose that the matrix were not invertible for some choice of the points then there is a non-zero vector $[V^T \quad W^T]$ such that

$$\begin{bmatrix} K & F \\ F^T & 0 \end{bmatrix} \begin{bmatrix} V \\ W \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{16}$$

Then $KV + FW = 0$ and $F^T V = 0$, the latter being condition (4) in the definition of positive definiteness. Now note that

$$[V^T \quad W^T] \begin{bmatrix} K & F \\ F^T & 0 \end{bmatrix} \begin{bmatrix} V \\ W \end{bmatrix} = V^T KV + V^T FW + W^T F^T V = V^T KV \tag{17}$$

but we see that (16) implies that $V^T KV = 0$. In turn this implies that $V = 0$ and finally $W = 0$ because the functions in K are lineraly independent.

Note that i. an estimator/interpolator is obtained that is exactly the same as a kriging estimator (but written in dual form) and ii. no probabilistic or smoothness conditions have been imposed. Moreover the interpolating function is non-unique in the sense that any function positive definite in the sense of Definition 1 will do. In the derivation of the kriging estimator there is a presumption that there is a unique generalized covariance (unique up to certain additive terms which do not effect the estimator) and hence one must search for at least an approximation to that unknown model. From the perspective of splines the non-uniqueness is removed by imposing certain smoothness conditions. In the literature on Radial Basis Functions there seems to be litle emphasis on the question of which Radial Basis Function to use or how it is selected.

4 - MOVING AVERAGES

Of course it is well-known that in one sense the Kriging estimator is simply a weighted average of the data and if a non-unique neighborhood is used then it is in fact a moving average. The key difference is in how the weights are assigned. This representation as a moving average appears in a different light if the kriging estimator is written in the dual form. Consider an interpolator in the form (15') with particular choices of the function g. If g is a covariance corresponding to a pure nugget then

$$\int f(y)g(x,y)dy = cf(x) \tag{18}$$

where c is the magnitude of the nugget. That is, g is the Dirac Delta function. g is an averaging function but its window consists of only one point. In contrast a covariance corresponding to a spherical variogram would have an averaging window of width two times the range. Exponential models have an effective window width that is finite as does the Gaussian but power models and generalized covariances in general have infinite window widths. In view of Bochner's theorem it is not surprising that the averaging functions are essentially probability densities. This formulation also appears in estimators of distribution functions. The empirical distribution corresponds to a nugget effect model but a number of authors have used averaging functions (i.e., probability densities to obtain improved distribution function estimators. Indicator Kriging is an example of such an approach although not always recognized as such. The choice of the generalized covariance (e.g., Radial Basis Function) then is characterized by the parameters of the window of the averaging function, its width and shape.

5 - USES AND QUESTIONS

While the typical application has been thought of as one in which the function is unknown and hence the optimal choice of the basis function is also unknown, Powell has proposed the use of such interpolators as computational aid for minimization (or maximization) of a function when analytical methods are not available or readily applicable. That is, one finds (approximations to) the critical point(s) on the given surface by finding the critical point(s) on the interpolated surface. This potential application suggests some new perspectives on the question of variogram modelling, in particular what are adequate and appropriate criteria for optimal modelling of the variogram (or generalized covariance)?

In the context of the derivation of the kriging estimator the question of the estimation of the variogram does not even appear, there is a presumption of its existence and the non-uniqueness of the generalized covariance due to additive polynomials does not affect the kriging estimator. As a consequence the emphasis has been on statistical approaches. In contrast the spline is obtained by imposing a smoothness condition on the interpolated surface but except at the data points no conditions are imposed on the quality of approximation. Perhaps the ultimate solution lies in a new formulation that incorporates both the approach suggested by the derivation of the spline as well as the minimum variance approach utilized in the derivation of the kriging estimator.

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