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NEW TYPES OF DISJUNCTIVE KRIGING

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INTRODUCTION

In the decade since the first paper on non-linear geostatistics appeared (Matheron, 1973), geostatisticians have had the time to test the method and find its strengths and weaknesses. One problem to date has been that, in its present form, disjunctive kriging has always been associated with a transformation to a normal distribution, which is unsuited for use with data like uranium, with a large peak of zero values, or with discrete variables such as the stone counts on diamonds or with grouped data as is found in size or density distributions. So there is a very real need for new types of disjunctive kriging, particularly for "discrete disjunctive kriging".

The first note on disjunctive kriging (Matheron, 1973) gives the theory behind the method and shows how it can be used for data having one of the following distributions: the normal distribution, the gamma, the Poisson and the negative binomial. More importantly, the general conditions for finding distributions suitable for disjunctive kriging are presented. These are that the joint distribution $f(x,y)$ can be expressed in an isofactorial form; that is,

$$f(x,y) = \sum_{n=0}^{\infty} T_n \chi_n(x) \chi_n(y) f_1(x) f_2(x)$$

where $f_1(.)$ is the marginal distribution, T_n are constants and $\chi_n(.)$ are the factors which, for simplicity, must be polynomials. A recent translation of this work is presented in a previous paper (Matheron and Armstrong, 1984).

One unfortunate limitation of this method for finding distributions suitable for disjunctive kriging was that it could only be applied to infinitely divisible distributions. This limitation can be overcome by using a different approach (infinitesimal generators).

This was first developed for continuous distributions (Matheron, 1975a) and afterwards to discrete distributions (Matheron, 1975b). The objective of this paper is to present an updated translation of those parts of these two research notes which are directly relevant to alternative types of disjunctive kriging.

The first of these two notes is a collection of rather disparate results which are not all concerned with the subject under discussion, and which will therefore not be presented in detail here. However, an overview of both papers will be given for the sake of completeness.

I - OVERVIEW OF THE FIRST NOTE.

The first note "Compléments sur les modèles isofactoriels" regroups some rather diverse results, as can be seen from the chapter headings:

1. A random set deduced from a Gaussian random function.
2. The general form of "Hermitian" distributions.
3. The general form of "Laguerre" distributions.
4. The covariance of an anamorphosis.
5. The infinitesimal generator approach.
6. The compactness of a family of isofactorial distributions.

In the first section, it is shown that if $Y(x)$ is a normally distributed random variable ($N(0,1)$) with spatial covariance of $\rho(x,y)$, then the covariance of the random set $A = \{x:Y(x) \geq a\}$ can be expanded in terms of Hermite polynomials as

$$C(x,y) = (1 - G(a))^2 + \sum_{n=1}^{\infty} (\rho(x,y))^n \frac{(H_{n-1}(a)\ g(a))^2}{n\ !}$$

where $g(.)$ and $G(.)$ are the p.d.f. of the standard normal distribution and the corresponding distribution function. It then goes on to show that if $\rho(x,y)$ is near 1 (that is, if $h = |x-y|$ is smaller and there is no nugget effect), the variogram corresponding to $C(x,y)$ is proportional to the square root of the variogram $(1 - \rho(h))$ of $Y(x)$. Consequently for the variogram of the random set to be linear near the origin, $1 - \rho(h)$ must be parabolic. So the covariance model for $\rho(h)$ would have to be like e^{-bh^2}.

The second and third sections are devoted to definitions of wider classes of bivariate distributions that have respectively the standard normal distribution (or the gamma distribution) as their marginal distribution and having Hermite (or Laguerre) polynomials as their orthogonal polynomials. For want of a better name, they were called "Hermitian" and "Laguerre"-type distributions. These are a generalisation of the bivariate normal and bivariate gamma distributions. In a course on non-linear geostatistics, Rivoirard (1984) pointed out that the Hermitian distributions may prove useful in handling anamorphosed uranium data which, by construction, has a normal distribution as its marginal distribution but which is often not a bivariate normal. Figure 1a presents a diagrammatic representation of the isoprobability curves for typical uranium data while Figure 1b represents a bivariate normal distribution.

As the same line of reasoning is used in both sections, the the first one (on the Hermitian distributions) will be presented in full but the details of the other will be left to the reader.

The objective of the fourth section is to extend some results on the covariance of an anamorphosed variable, which Maréchal (1975) has obtained.

By far the most important section is the fifth one which uses infinitesimal generators to produce isofactorial models with polynomial factors for continuous distributions. In addition to the Hermite and Laguerre-type distributions, the beta distribution is shown to be suitable for disjunctive kriging. (The corresponding factors are the Jacobi polynomials). The theory developed in this section demonstrates that the isofactorial models with polynomial factors belong to the family of semi-groups associated with diffusion type processes. More recently, Matheron (1983) has presented some change of support models for these diffusion-type processes.

In the last section, it is shown that the families of isofactorial distributions are closed and compact.

2 - OVERVIEW OF THE SECOND NOTE.

One limitation of the first note was that it dealt only with continuous distributions. This is overcome by the second one which treats discrete distributions. The infinitesimal generators are used to obtain isofactorial models with polynomial factors for the binomial, Poisson, negative binomial and hypergeometric distributions. As with Section 5 of the preceding note, a full translation of the work is given.

The second half of the note introduces a bivariate form of Walsh's distribution which also has polynomial factors. Walsh's process X(t) is

$$X(t) = \sum_{1}^{\infty} \frac{\varepsilon_n(t)}{2^n}$$

where the $\varepsilon_n(t)$ form a two state (0 or 1) Markov chain with the transition matrix

$$\begin{pmatrix} \frac{1+\rho}{\alpha} & \frac{1-\rho}{2} \\ \frac{1-\rho}{2} & \frac{1+\rho}{2} \end{pmatrix} \quad \text{where } \rho = e^{-t}$$

Walsh's process is Markovian but its transition matrix cannot be expressed in a simple way because the transition probabilities are continuous but not absolutely continuous.

At the end of the note, a link is established between de Wijsian random variables and a generalisation of this process to the case where the correlation coefficient ρ is a random variable instead of being deterministic.

As possible applications for this model are somewhat limited, this section will not be presented in detail.

We now present translations of sections directly related to disjunctive kriging; viz

* the Hermitian distributions
* the Infinitesimal Generator approach used with continuous distributions
* the Infinitesimal Generator approach used with discrete distributions.

3 - THE GENERAL FORM OF HERMITIAN DISTRIBUTIONS.

When the correlation coefficient ρ of a bivariate normal distribution $G_\rho(dx,dy)$ takes the value 1, $G_\rho(dx,dy)$ is no longer a cumulative distribution function. However the relation

$$E[H_n(X)|Y] = \rho^n H_n(Y)$$

is still valid. It is interesting to generalize the bivariate normal distribution to include this case and others.

A distribution $F(dx,dy)$ is said to be a Hermitian distribution if it satisfies the following two conditions :

1. The marginal distributions are all standard normal distributions.
2. The Hermite polynomials satisfy :

$$\left\{ \begin{array}{l} E[H_n(X)|Y] = T_n \; H_n(Y) \\ E[H_n(Y)|Y] = T_n \; H_n(X) \end{array} \right. \quad \text{for } n = 0,1,\ldots \qquad (1)$$

This condition means that T_n is the correlation coefficient between the normed Hermite polynomials $\eta_n(X)$ and $\eta_n(Y)$, and consequently that

$$T_o = 1$$

and

$$|T_n| \leq 1.$$

Even if these conditions are satisfied, it is not clear that a sequence of coefficients T_n should be unique. We now establish the necessary and sufficient conditions for this.

<u>THEOREM</u>. A sequence of coefficients T_n is associated with a Hermite distribution if

$$T_n = \int \rho^n \ \omega(d\rho) \qquad (2)$$

where $\omega(d\rho)$ is a distribution function concentrated on the closed interval $[-1,+1]$ and the T_n are unique.

This condition is clearly sufficient since if the condition holds, the Hermitian distribution is a random mixture of normal distributions obtained by letting ρ vary according to a distribution ω. It is defined by its characteristic function :

$$\Phi(U,V) = \int e^{-\frac{1}{2}(U^2+V^2+2\rho UV)} \ \omega(d\rho)$$

$$= e^{-\frac{1}{2}(U^2+V^2)} \ \Sigma \frac{\rho^n}{n!} \ (iU)^n \ (iV)^n$$

We now show that this condition is also necessary. Let F be a Hermitian distribution. From the relation (established in Matheron 1975a)

$$e^{-\lambda x+\lambda^2/2} = \Sigma \ (-1)^n \ \frac{\lambda^n}{n!} \ H_n(x)$$

it follows that

$$e^{\lambda^2/2} \ E[e^{-\lambda X} | Y=y] = \Sigma \ \frac{(-1)^n}{n!} \ T_n \ \lambda^n \ H_n(y)$$

The left-hand term is non-negative. Moreover $e^{\lambda^2/2} \ E(e^{\lambda X} | Y=y) \ G(dy)$ is a probability. So is the expression

$$\Sigma \ \frac{(-1)^n}{n!} \ T_n \ \lambda^n \ H_n(y) \ G(dy) \qquad (3)$$

Provided that $T_o = 1$ and $T_n \leq 1$ we can take the Fourier Transform and get a characteristic function.

$$\varphi_\lambda(U) = \Sigma \ \frac{(-1)^n}{n!} \ T_n \ \lambda^n \quad e^{iVy} \ H_n(y) \ G(dy)$$

Moreover since

$$\int_{-\infty}^{\infty} e^{iUy} H_n(y)\ G(dy) = (-1)^n (iU)^n e^{-U^2}$$

we have

$$\Phi_\lambda(U) = \Sigma\, T_n \frac{\lambda^n}{n!} (iU)^n e^{-U^2/2}$$

Replacing U by t/λ and letting λ tend to infinity gives

$$\lim_{\lambda\to\infty} \Phi_\lambda \left(\frac{t}{\lambda}\right) = \Sigma\, T_n \frac{(it)^n}{n!}$$

As this limit is a continuous function of t (since $|T_n| \leq 1$), the resulting function is still a characteristic function. (The positivity is clearly preserved when going to the limit). There is, therefore, a distribution ω such that

$$\Sigma\ T_n \frac{(it)^n}{n!} = \int e^{it\rho}\ \omega(d\rho)$$

Hence

$$T_n = \int \rho^n\ \omega(d\rho)$$

Moreover since $|T_n| \leq 1$, this distribution has to be concentrated on the closed interval $[-1,+1]$. Finally, since ω is concentrated on a bounded interval, it is uniquely determined by its moments. (See Kendall and Stuart, Vol. I, pp. 89-90). Consequently the Hermitian distribution F is unique.

In addition to this, these distributions form a closed convex set which is compact under convergence in distribution. (The convergence of a sequence of Hermitian distributions F_n is equivalent to that of the associated distributions $\omega_n(d\rho)$ and so the distributions form a compact set).

- NOTE 1 - As was indicated in the introduction, a similar result can be proved for the "Laguerre"-type distributions which bear the same relation to the gamma distribution as the Hermitian distribution does to the normal. One slight difference is that as the gamma distribution is defined on R+, the correlation coefficient between the orthogonal polynomials ρ must be positive, and consequently

$$T_n = \int_0^1 \rho^n \, \omega(d\rho) \qquad (4)$$

This is not the first time that this relation (4) has appeared with gamma processes. It also arose in the form

$$T_n = E[X^n]$$

where X had a beta distribution $(\rho\alpha, (1-\rho)\alpha)$ with mean ρ, in Matheron (1973).

More recently (Matheron (1983)), it also was proved for the negative binomial distribution :

$$T_n = \int_0^1 \rho^n \, \omega(d\rho)$$

What is even more interesting, an equivalent result was also established for the asymmetric bivariate distribution (i.e. the point-block distribution) which is essential for change of support.

4 - THE INFINITESIMAL GENERATOR METHOD APPLIED TO CONTINUOUS DISTRIBUTIONS.

The principal aim of this paper and of the preceding one is to follow the development of alternative types of disjunctive kriging. In Part I of this paper, four distributions (normal, gamma, Poisson and negative binomial) were shown to have the required isofactorial properties together with polynomial factors. Unfortunately the method used for finding suitable models could only be used with infinitely divisible distributions.

Here infinitesimal generators and the theory of semi-groups are used to find other suitable models. In this section, the method is applied to continuous distributions; the discrete case is treated in the following one. In both cases we give only an outline of the proof. Readers who wish to fill out the proof may find it helpful to consult a text on functional analysis (such as Brezis (1983)), in particular for the Hille-Yosida theorem.

Let $g(x)$ be the marginal distribution. Working in the space $L^2(\mathbb{R},g)$, we want to find a function $a(x)$ so as to write the differential operator Af associated with the stochastic process in the form

$$Af = af'' + \frac{f'}{g}\frac{d}{dx}(ag)$$

where $f' = \frac{\partial f_t}{\partial t}$.

Provided that $a(x)$ and $g(x)$ are regular enough in the domain of definition of $g(x)$ and that their product goes to zero at the limits of this (which is the case in practice), then integration by parts can be used to show that

$$\int a(x)\, f''(x)\, g(x)\, \varphi(x)\, dx + \int \frac{f'(x)}{g(x)}\frac{d}{dx}(a(x)\, g(x)\, g(x)\, \varphi(x)\, dx$$

$$= - \int f'(x)\, a(x)\, g(x)\, \varphi'(x)\, dx$$

So

$$Af = af'' + \frac{f'}{g}\frac{d}{dx}(ag)$$

$$= \frac{1}{g}\frac{d}{dx}(agf')$$

That is, the evolution equation:

$$\frac{\partial f_t}{\partial t} = Af = \frac{1}{g}\frac{\partial}{\partial x}\left[ag\frac{\partial f_t}{\partial t}\right] \qquad (5)$$

is a type of heat equation. The operator A is a negative Hermitian operator (in the sense that the scalar product $\langle Af, f\rangle = -\langle \sqrt{a}\, f', \sqrt{a}\, f'\rangle \leq 0$.

Now provided that A is closed and dense in $L^2(\mathbb{R},g)$ there exists a semi-group $P_t = e^{At}$ with A as its infinitesimal operator, and since we are dealing with a heat equation, this is a diffusion semi-group. From (5), $\int g\, A f_t = 0$ and so the density g is the ergodic limit of $P_t(x;dy)$ as $t \to \infty$.

The next step is to see whether the eigen functions associated with the operator A include a series χ_n which forms an orthonormal basis for $L^2(\mathbb{R},g)$. If this is the case, then

$$P_t\, \chi_n = e^{-\lambda_n t}\, \chi_n$$

where λ_n is the eigen value corresponding to χ_n.

Consequently for any function $f \in L^2(\mathbb{R},g)$

$$P_t\, f = \sum e^{-\lambda_n t} < f, \chi_n > \chi_n$$

The bivariate distribution $F_t(dx,dy) = g(x)\; P_t(dx,dy)\; dx$ can therefore be written in an isofactorial form :

$$F_t(dx,dy) = \sum e^{-\lambda_n t}\; \chi_n(x)\; \chi_n(y)\; g(x)\; g(y)\; dx\; dy.$$

In other words, the Markov process associated with this semi-group is an isofactorial model.

A few examples should help clarify this approach.

1. <u>Gaussian Process on the whole line</u>.

This corresponds to the case $a(x) = 1$ and $g(x) = \frac{1}{\sqrt{a\Pi}}\, e^{-x^2/2}$. Here

$$A\, f = f'' - x\, f'$$

which is clearly equal to $\frac{1}{g}\frac{d}{dx}(g\, f')$. The orthogonal polynomials relative to the normal distribution are the Hermite polynomials $H_n(x)$.

Moreover, since $A H_n = -n H_n$, the eigen values are $\lambda_n = n$ and so the bivariate distribution $F_t(dx,dy)$ is $\Sigma \rho^n H_n(x) H_n(y) g(x) g(y) dx dy$ where the correlation coefficients ρ equals e^{-nt}.

2. The Gamma Process on R^+.

This time $a(x) = x$ and $g(x) = \frac{1}{\Gamma(\alpha)} x^{\alpha-1} e^{-x}$.

Consequently,

$$Af = x f'' + (\alpha-x) f'$$

The Laguerre polynomials

$$L(-n,\alpha,x) = 1 + \sum_{k=1}^{n} \frac{(-1)^k n(n-1) \dots (n-k+1) x^k}{\alpha(\alpha+1) \dots (\alpha+k-1) k!}$$

are the eigen functions associated with the eigen value $-\lambda_n = -n$. Letting ℓ_n denote the normed polynomial, the representation for the bivariate distribution is then

$$F_t = \Sigma e^{-nt} \ell_n(x) \ell_n(y) x^{\alpha-1}_{\Gamma(\alpha)} y^{\alpha-1}_{\Gamma(\alpha)} e^{-x-y}$$

- NOTE 1 - The definition given here for the Laguerre polynomials is not the same as in earlier notes. They differ by a multiplicative factor $(-1)^n(\alpha+n-1)(\alpha+n-2) \dots \alpha$. The new definition is used because it considerably simplifies the form of the recurrence relation used to a Laguerre polynomial from the preceding two polynomials.

3. Beta Process on (0,1).

In this case $a(x) = x(1-x)$

and

$$g(x) = \frac{\Gamma(\alpha+\beta) x^{\alpha-1}(1-x)^{\beta-1}}{\Gamma(\alpha) \Gamma(\beta)} \qquad 0 \le x \le 1$$

5 - THE INFINITESIMAL GENERATOR METHOD APPLIED TO DISCRETE DISTRIBUTIONS.

In the preceding section it was shown how isofactorial models with polynomial factors could be found for continuous distributions from Markov processes where the infinitesimal generator was local. In this section, similar models are obtained for discrete distributions. The local nature of the infinitesimal generator A is replaced by a condition limiting possible transitions to adjoining states, that is $i \to i+1$ or $i \to i-1$. Consequently

$$(Af)i = -(a_i + b_i)f_i + a_i f_{i+1} + b_i f_{i-1} \qquad (6)$$

where a_i is the probability of the transition $i \to i+1$ and b_i is the probability of the transition $i \to i-1$.

Three different types of processes can be distinguished, depending on the values of a_i and b_i.

1. If a_i and b_i are strictly positive for $i = 0, \pm 1, \pm 2, \ldots$, i can vary from $-\infty$ to $+\infty$. This case will not be treated here (the reasons for this choice become apparent in the next paragraph).
2. If $b_o = 0$ and $b_i > 0$ for $i = 1, 2, \ldots$, and $a_i > 0$ for all i, then i varies from 0 to ∞ (infinite case).
3. If $b_o = 0$ and $a_N = 0$, and if $b_i > 0$ for $i = 1, \ldots.$ N and $a_i > 0$ for $i = 0, \ldots N-1$, then i varies from 0 to N (finite case).

In addition to this, the process must be ergodic, so there must be a probability $W = \{w_i\}$ such that

$$-(a_i + b_i) w_i + a_{i-1} w_{i-1} + b_{i+1} w_{i+1} = 0$$

On re-writing this as

$$b_{i+1} w_{i+1} - a_i w_i = b_i w_i - a_{i-1} w_{i-1}$$

it is clear that

$$b_{i+1} + w_{i+1} = a_i \, w_i \qquad (7)$$

If a_i and b_i are strictly positive, (7) is true provided that $a_i \, w_i$ and $b_i \, w_i$ tend to 0 as i tends to $-\infty$. However in the two cases of interest to us (the finite and infinite cases), we have $b_o = 0$ and so (7) is true. No additional hypotheses are required. Therefore the limiting distribution (if it exists) is defined by

$$w_n = \frac{a_o}{b_1} \frac{a_1}{b_2} \cdots \frac{a_{n-1}}{b_n} w_o \qquad (8)$$

and so the condition for its existence is that $\Sigma \, w_n < \infty$.

Condition (7) also means that the process is reversible, since $w_i \, P_{ij}(t) = w_j \, P_{ji}(t)$ (where $P_{ij}(t)$ is the probability of going from i to j in time t).

5.1 <u>Condition for Polynomial Factors</u>.

Since the process is reversible, there will be polynomial factors if and only if

I. The polynomials belong to $L^2(\mathbb{R},W)$; that is

$$E(i^n) = \sum w_i \, i^n < \infty$$

II. For each n, A_i^n is a polynomial of degree n in i (where $n = 0, 1, 2 \ldots \infty$ or $n = 0, 1, \ldots N$ as the case may be).

Taking condition II first,

$$A_i^n = a_i[(i+1)^n - i^n] + b_i[(i-1)^n - i^n]$$

So for n = 1

$$A_i = a_i - b_i$$

and this must be 1st degree polynomial in i.

For n = 2

$$A_i^2 = a_i[2i+1] + b_i[-2i+1]$$

and this must be a 2nd degree polynomial in i.

These two conditions are satisfied if

$a_i - b_i$ is linear and

$a_i + b_i$ is quadratic

that is, if a_i and b_i are of the form

$$a_i = a_o + \alpha_i + \gamma_i^2$$
$$b_i = b_o + \beta_i + \gamma_i^2 \qquad (9)$$

Moreover $b_o = 0$ since we are not concerned with cases where i goes from $-\infty$ to ∞. It is easy to see that if a_i and b_i are of this form, condition (7) is satisfied for all n.

It remains to show that condition I is also satisfied in the infinite case. (It obviously is for the finite one). In the case where a_i and b_i are both strictly positive, i.e. where i varies from $-\infty$ to $+\infty$, we find that $E[i^n] = \infty$ for sufficiently large n and consequently that there are no models with polynomial factors. This is why this case has not been considered .

5.2 Linear Models : $\gamma = 0$

Here $a_i = a_o + \alpha_i$

$b_i = \beta_i$

Now a_o must be strictly positive or else the process stops, and similarly so must β. There are three cases to consider : $\alpha > 0$, $\alpha = 0$, $\alpha < 0$, which lead respectively to the negative binomial, the Poisson, and the binomial distributions. (This progression is hardly surprising when the limit relations between the different distributions are remembered).

(i) <u>Case $\alpha > 0$: Negative Binomial Distribution.</u>

From (8), it is clear that

$$W_n = \left(\frac{\alpha}{\beta}\right)^n \left[\frac{a_o}{\alpha}\left(\frac{a_o}{\alpha} + 1\right) \cdots \left(\frac{a_o}{\alpha} + n-1\right)\right] \frac{W_o}{n!}$$

Putting $p = \frac{\alpha}{\beta}$, $\nu = \frac{a_o}{\alpha}$

$$\sum w_n s^n = (1 - ps)^{-\nu} W_o \qquad s < \frac{1}{p}$$

Therefore the limiting distribution W exists iff $p < 1$, that is if $\alpha < \beta$. In that case, the generating function is

$$G(s) = \frac{q^\nu}{(1 - ps)^\nu}$$

where $q = 1-p$. Since G(s) can be differentiated as many times as is desired, the polynomials belong to $L^2(\mathbb{R},W)$. Provided $\alpha < \beta$, there is therefore an isofactorial model with polynomial factors and with the negative polynomial

$$W_n = q^\nu \frac{\Gamma(\nu+n)}{\Gamma(\nu)} \frac{p^n}{n!}$$

as its marginal distribution.

The polynomials now have to be determined explicitely. To do this, we need the eigen values of the operator A, which can be found by finding the coefficient of i^n in the expression for A_i^n

$$A_i^n = (a_o + \alpha_i) [(i+1)^n - i^n] - \beta_i[i^n - (i-1)^n]$$

$$= n(\alpha - \beta) i^n + \text{polynomial of degree} < n.$$

Consequently

$$\lambda_n = - n(\beta - \alpha) = - n\beta q$$

So if we let $\chi_n(i)$ denote the normed factor of degree n, the bivariate distribution $F_{ij}(t)$ is

$$F_{ij}(t) = W_i \; W_j \sum_{n=0}^{\infty} \rho^n \; \chi_n(i) \; \chi_n(j) \tag{10}$$

where $\rho = e^{-\beta q t}$.

Moreover

$$F_{ij}(t) = W_i \; P_{ij}(t)$$

where $P_{ij}(t)$ is the transition matrix which is the resolution of the second Kolmogorov equation :

$$\frac{d}{dt} P_{ij}(t) = -(a_j + b_j) \; P_{ij}(t) + a_{j-1} \; P_{ij-1}(t) + b_{j+1} \; P_{j+1}(t) \tag{11}$$

Putting

$$b_i(s,t) = \sum_j P_{ij}(t) \; s^j$$

equation (10) then becomes

$$\frac{\partial G}{\partial t} + (1 - s)(\alpha s - \beta) \frac{\partial b}{\partial s} = -a_o(1 - s)$$

with $G_i(s,\sigma) = s^i$. Integrating this gives

$$G_i(s,t) = \left(\frac{(1 - ps - \rho(1-s)}{1 - ps \; p\rho(1-s)}\right)^i \left(\frac{q}{1 - ps - p\rho(1-s)}\right)^\nu \tag{10}$$

The bivariate generating functions in terms of s and σ (t is implicit) can be deduced from (11)

$$\begin{aligned} G(s,\sigma) &= \sum_{i,j} F_{ij} \; s^j \; \sigma^i \\ &= \sum W_i \; \sigma^i \; G_i(s,t) \\ &= \left(\frac{q^2}{(1-ps)(1-p\sigma) - \rho \; p(1-s)(1-\sigma)}\right)^\nu \end{aligned}$$

This can be expanded in terms of ρ as

$$G(s,\sigma) = \left(\frac{q^2}{(1 - ps)(1 - p\sigma)}\right)^{\nu} \sum_{0}^{\infty} \frac{\Gamma(\nu+n)\ p^n \rho^p}{\Gamma(\nu)\ n!} \frac{(1 - s)^n (1 - \sigma)^n}{(1 - \rho s)^n (1 - \rho\sigma)^n}$$

From (10) we also have

$$G(s,\sigma) = \sum_n \rho^n \sum_i W_i\ \chi_n(i)\ s^i \sum_j W_j\ \chi_n(j)\ \sigma^j$$

Since $\rho = e^{-\beta q t}$ varies from 0 to ∞, we can equate the terms in these two expansions. This shows that the generating function of the $\chi_n(i)W_i$ is

$$\sum\ \chi_n(i)\ W_i\ s^i = q^{\nu} \sqrt{\frac{\Gamma(\nu+n)\ p^n}{\Gamma(\nu)\ n!}}\ \frac{(1 - s)^n}{(1 - ps)^{n+\nu}}$$

The polynomial $\chi_n(i)$ can be deduced from this to be

$$\left[\frac{\Gamma(\nu+n)}{\Gamma(\nu)}\ \frac{p^n}{n!}\right]^{1/2} \sum_{k=0}^{n} (-1)^k\ \frac{{}^nC_k\ \Gamma(\nu+i+n-k)}{\Gamma(\nu+i)}\ \frac{i(i-1)\ \dots\ (i-k+1)}{p^k}$$

(ii) <u>Case $\alpha = 0$: Poisson Distribution.</u>

If $\alpha = \gamma = b_o = 0$ in (9), then $a_i = a_o$ and $b_i = \beta_i$ where $\beta > 0$. From (8) the limiting distribution still exists and is a Poisson distribution with parameter $\theta = \frac{a_o}{\beta}$. The corresponding stochastic process describes a queueing process with an infinite number of servers, when the arrival times follow a Poisson distribution with parameter a_o and the service time distribution is exponential with parameter β. The infinitesimal generator is

$$(Af)_i = a_o(f_{i+1} - f_i) - \beta_i(f_i - f_{i-1})$$

Consequently the eigen value λ_n associated with the polynomial factor χ_n (of degree n) $\lambda_n = - n\beta$.

So the bivariate distribution $F_{ij}(t) = W_i \; P_{ij}(t)$ can be written as

$$F_{ij} = W_i \; W_j \sum_{n=0}^{\infty} \rho^n \chi_n(i) \; \chi_n(j) \qquad (12)$$

where $\rho = e^{-\beta t}$.

Using Kolmogorov's second equation, it is not difficult to show that

$$\sum_j P_{ij}(t) \; s^j = (1 - \rho + p\rho)^j \; e^{-\theta(1-\rho)(1-s)}$$

and hence to deduce the generating function for the bivariate distribution :

$$\begin{aligned} G(s,\sigma) &= \sum_{ij} F_{ij} \; s^j \; \sigma^j \\ &= \sum_{ij} W_i \; P_{ij} \; \sigma^i \; s^j \\ &\doteq e^{-\theta(1-s) \; - \; \theta(1-\sigma) \; + \; \rho(1-s)(1-\sigma)} \end{aligned}$$

We now compare this with the expression for the generating function obtained from (12)

$$G(s,\sigma) = \sum_n \rho^n \sum_i W_i \; \chi_n(i) \; \sigma^i \sum_j W_j \; \chi_n(j) \; s^j$$

Identifying the coefficients of the terms in ρ^n gives

$$\begin{aligned} \sum W_i \; \chi_n(i) \; s^i &= \sqrt{\frac{\theta^n}{n!}} \; (1-s)^n \; e^{\theta(1-s)} \\ &= (-1)^n \sqrt{\frac{\theta^n}{n!}} \; \frac{d^n}{d\theta^n} \; e^{\theta(1-s)} \end{aligned}$$

Consequently

$$W_i \; \chi_n(i) = (-1)^n \sqrt{\frac{\theta^n}{n!}} \; \frac{d^n}{d\theta^n} \left(\frac{\theta^i}{i!} \; e^{-\theta} \right)$$

Therefore

$$\chi_n(i) = (-1)^n \sqrt{\frac{\theta^n}{n!}} \; \frac{i!\, e^{\theta}}{\theta^i} \; \frac{d^n}{d\theta^n}\left(\frac{\theta^i}{i!}\, e^{-\theta}\right)$$

(iii) Case $a < 0$: Binomial Distribution.

If α is negative, $a_i = a_o + \alpha_i$ would become negative for sufficiently large values of i. As $\{i\}$ must therefore be finite, a_i must be zero for some value of $i = N$ and the process is restrained to the interval $(0,N)$. We therefore have

$$a_i = a(N-i) \;, \quad b_i = bi$$

From (8), the limiting distribution is a binomial distribution with parameters p and N where

$$p = \frac{a}{a+b}$$

The infinitesimal generator is

$$(Af)_i = a(N-1)\;[f_{i+1} - f_i] - bi[f_i - f_{i-1}]$$

and so the eigen value associated with χ_n is

$$\lambda_n = -\,n(a+b)$$

Consequently the bivariate distribution is

$$F_{ij}(t) = W_i \; W_j \sum \rho^n \; \chi_n(i) \; \chi_n(j) \tag{13}$$

where $\rho = e^{-(a+b)c}$ and $W_i = \binom{N}{i} p^i \;(1-p)^{N-i}$

The expression for $\sum_{j=0}^{\infty} P_{ij}(t)\, s^j$ can also be obtained directly to be

$$[q(1-\rho) + (p+\rho q)s]^i \; [q + \rho p + p(1-\rho)s]^{N-i}$$

where $q = 1 - p$.

Consequently

$$G(s,\sigma) = \sum W_i P_{ij}(t) s^j \sigma^i$$

$$= [(q+ps)(q+p\sigma) + \rho pq(1-s)(1-\sigma)]^N$$

Expanding this in powers of ρ gives

$$G(s,\sigma) = (q + ps)^N(q + p\sigma)^N \sum_o^\infty \rho^n p^n q^n \frac{N}{n} \left[\frac{(1-s)(1-\sigma)}{(q+ps)(q+p\sigma)}\right]^n$$

Another expression for $G(s,\sigma)$ can be obtained directly from (13). Identifying the terms in the two expressions gives

$$\sum W_i \chi_n(i) s^i = \sqrt{\binom{N}{n} p^n q^n} (1-s)^n(q+ps)^{N-n}$$

$$= \frac{n!}{N!}\sqrt{\binom{N}{n} p^n q^n} \frac{d^n}{dq^n} [q(1-s) + s]^N$$

Consequently

$$W_i \chi_n(i) = \frac{n!}{N!}\sqrt{\binom{N}{n} p^n q^n} \frac{d^n}{dq^n} \left[\binom{N}{i} (1-q)^i q^{N-i}\right]$$

Hence

$$\chi_n(i) = \sqrt{\frac{n! p^n q^n}{N! (N-n)!}} \frac{1}{(1-q)^i q^{N-i}} \frac{d^n}{dq^n} [q^{N-i}(1-q)^i]$$

We now consider the case where γ is not zero.

(iv) <u>Case $\gamma \neq 0$: Hypergeometric Distribution.</u>

In this case,

$$a_i = a_o + \alpha_i + \gamma_i^2$$

$$b_i = \beta_i + \gamma_i^2$$

where $\gamma \neq 0$. In the infinite case $\gamma > 0$, $a_o > 0$ and a_i, $b_i > 0$ for i = 1, 2, ... , it is possible to obtain a limiting distribution W provided that certain conditions are satisfied but even then the polynomials of degree n need not belong to $L^2(R,W)$ when n becomes large. Consequently there are no polynomial factors.

However in the finite case, there is a solution. Suppose $0 \le i \le N$. Then, changing the notation slightly we have

$$a_i = (N-i)\,[a + \gamma(N-i)]$$
$$b_i = i[b + \gamma i]$$

where $a + \gamma > 0,\ a + N\gamma > 0\ ;\ \ b + \gamma > 0,\ b + N\gamma > 0$

From (8), the limiting distribution is of the form

$$W_n = \frac{N(N-1)\ \dots\ (N-n+1)}{n!}\ \frac{(\frac{a}{\gamma} + N)\dots(\frac{a}{\gamma} + N - n+1)}{(1 + \frac{b}{\gamma})\ \dots\ (n + \frac{b}{\gamma})}\ W_o$$

Putting $\frac{a}{\gamma} + N = \alpha$ and $\frac{b}{\gamma} = \beta$ gives

$$W_n = \frac{(-N)\ \dots\ (-N+n-1)}{n!}\ \frac{(-\alpha)(-\alpha+1)\ \dots\ (-\alpha+n-1)}{\beta(\beta+1)\ \ (\beta+n-1)}\ W_o$$

Since $\Sigma\, W_n = 1$,

$$W_o = \frac{\Gamma(\alpha+N)\ \Gamma(\beta+N)}{\Gamma(\beta)\ \Gamma(\alpha+\beta+N)}$$

Hence

$$W_n = \binom{N}{n}\frac{\Gamma(\beta+N)\ \Gamma(\alpha+N)}{\Gamma(\beta+n)\ \Gamma(\alpha+\beta+N)}\ \alpha(\alpha-1)\ \dots\ (\alpha-n+1)$$

The polynomial factors still have to be found explicitly, but as this is much more complicated than in the preceding cases, it will be left till it is needed for practical applications.

CONCLUSION.

The isofactorial models presented in this paper and its predecessor make it possible to carry out disjunctive kriging when the data is not normally distributed. Continuous distributions such as the gamma and the beta may be very useful for modelling long-tailed distributions, thus obviating the need for an anamorphosis as used in traditional Gaussian disjunctive kriging. The discrete isofactorial models have a wide range of potential uses with discrete data or grouped data. Only experience will show how useful they really are in practice.

Before concluding, it is important to point out to potential users, two limitations in the work presented in this paper. The first is of a numerical nature. While it is all very well to have isofactorial models with polynomial factors, these are of little practical interest unless the polynomials can be calculated quickly and efficiently. Some sort of recurrence relation is therefore needed. These exist and can be found in any standard reference on orthogonal polynomials.

The second limitation concerns the "change of support". One of the great advantages of the normal distribution is that it facilitated models of change of support, which are needed for the point-block models and block-block models. In this work, nothing is said about how these can be developed for these isofactorial models. Interested readers can consult some recent work (Matheron (1980), (1983), (1984)).