

Properties and simulation of α -permanental random fields

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Abstract

An α -permanental random field is briefly speaking a model for a collection of random variables with positive associations, where α is a positive number and the probability generating function is given in terms of a covariance or more general function so that density and moment expressions are given by certain α -permanents. Though such models possess many appealing probabilistic properties, many statisticians seem unaware of α -permanental random fields and their potential applications. The purpose of this paper is first to summarize useful probabilistic results using the simplest possible setting, and second to study stochastic constructions and simulation techniques, which should provide a useful basis for discussing the statistical aspects in future work. The paper also discusses some examples of α -permanental random fields.

Keywords: α -determinant; α -permanent; covariance; doubly stochastic construction; negative binomial distribution; perfect simulation; Poisson randomization.

1 Introduction

Permanental (or boson) and determinantal (or fermion) point processes as introduced by (Macchi, 1971, 1975) and their extensions to α -permanental and α -determinantal point processes (Shirai and Takahashi, 2003a,b, Georgii and Yoo, 2005, Hough *et al.*, 2006, McCullagh

and Møller, 2006) have in recent years been of much research interest in probability theory, with applications in statistical physics (here α is a positive parameter in the α -permanental case, while $1/\alpha$ is a negative integer in the α -determinantal case). However, to the best of our knowledge, the statistical and computational aspects of these models have so far mainly been unexplored, and many statisticians may be unaware of the models many appealing properties and potential applications. The focus of the present paper is on α -permanental point process models in the simplest setting, namely when such point processes can be identified by a random field $\mathbf{N} = (N_s; s \in S)$ of discrete non-negative random variables, where at first S is taken as a finite index set $S = \{s_1, \dots, s_m\}$, but extensions to infinite S is considered in the final part of the paper. We call such a random field an α -permanental random field. The present paper should provide a useful basis for discussing the statistical aspects of α -permanental random fields, and it is based partly on the above-mentioned references and the seminal work by Griffiths (1984), Griffiths and Milne (1987), and in particular Vere-Jones (1997), and partly on some new results of our own. Though many results extend to the general setting where S is a Polish space, including the special case of spatial point processes in \mathbb{R}^d , a much more technical exposition would then be needed, see e.g. Shirai and Takahashi (2003a).

Section 2 introduces some notation and discusses the definition and existence of α -permanental random fields, and in Section 3 some properties are explored. The stochastic construction and simulation of α -permanental random fields is covered in Section 4. In Section 5 specific examples of model types and some of their properties are presented. Finally, Section 6 discusses possible extensions of the models.

2 Preliminaries

2.1 Definition and notation

An α -permanental random field is specified by a real parameter $\alpha > 0$ and a function $C : S \times S \rightarrow \mathbb{R}$, which since S is finite can be identified with a real $m \times m$ matrix, also denoted C . Whether C is considered a function or a matrix will depend on the context, and the two representations are used interchangeably throughout the paper. Notationally we write $C_{i,j} = C(s_i, s_j)$. We define an α -permanental random field through its probability generating function as follows, where I denotes the identity matrix, $|A|$ is the determinant of a square matrix A , and we take $0^0 = 1$.

Definition 1 *Let $S = \{s_1, \dots, s_m\}$ be an arbitrary finite set, $\alpha > 0$, and $C : S \times S \rightarrow \mathbb{R}$. A collection of non-negative integer-valued random variables $\mathbf{N} = (N_s, s \in S)$ is said to be an α -permanental random field with parameter (α, C) if the probability generating function for \mathbf{N} ,*

$$\varphi(\mathbf{z}) = \varphi(z_s; s \in S) = E \prod_{s \in S} z_s^{N_s}$$

is of the form

$$\varphi(\mathbf{z}) = |I + \alpha(I - Z)C|^{-1/\alpha} \tag{1}$$

where Z denotes the diagonal matrix with $(z_s; s \in S)$ on the diagonal. We denote this $\mathbf{N} \sim \text{per}(\alpha, C)$.

In accordance with the references given at the very beginning of Section 1, we call it an α -permanental random field, while a so-called α -determinantal random field appears if α is negative (see Section 6.2). The reason for the names of these models are partly explained by

the close connection between α -determinants and α -permanents and the fact that density and moment expressions are given in terms of α -determinants or α -permanents, see Section 3.

For notational convenience we also write $N_{s_i} = N_i$. If $\mathbf{N} \sim \text{per}(\alpha, C)$ then $I + \alpha C$ is necessarily non-singular (otherwise (1) would not be well-defined for $\mathbf{z} = \mathbf{0}$), and we can define the matrix

$$\tilde{C} = \alpha C(I + \alpha C)^{-1} = I - (I + \alpha C)^{-1}. \quad (2)$$

Using this parameterization we can write (1) as

$$\varphi(\mathbf{z}) = \left[|I - \tilde{C}| / |I - Z\tilde{C}| \right]^{1/\alpha}. \quad (3)$$

On the other hand, if (3) is a probability generating function then $I - \tilde{C}$ is necessarily non-singular, and setting

$$C = \frac{1}{\alpha} \tilde{C}(I - \tilde{C})^{-1} \quad (4)$$

we obtain (1). Consequently, we can equally well parameterize $\text{per}(\alpha, C)$ by (α, \tilde{C}) .

Using the Schur decomposition of C (Bhatia, 1997), the relation between the eigenvalues λ_i of C and the eigenvalues $\tilde{\lambda}_i$ of \tilde{C} is seen to be

$$\lambda_i = \frac{\tilde{\lambda}_i}{\alpha - \alpha\tilde{\lambda}_i}, \quad \tilde{\lambda}_i = \frac{\alpha\lambda_i}{1 + \alpha\lambda_i}, \quad i = 1, \dots, m. \quad (5)$$

We let $\|\lambda_i\|$ denote the modulus of λ_i and define the spectral norm of C as

$$\|C\| = \max\{\|\lambda_1\|, \dots, \|\lambda_m\|\} \quad (\text{and similarly for } \tilde{C}).$$

2.2 Existence of the α -permanental random field

By Definition 1, $\text{per}(\alpha, C)$ exists if and only if (1) (or equivalently (3)) is a proper probability generating function. It is clear that this is not the case for all (α, C) . The problem of

characterizing the set of (α, C) such that (1) is a proper probability generating function is treated in detail in Vere-Jones (1997), but no easily verifiable necessary and sufficient condition is known. There are however some known sufficient conditions expressed either through (α, C) or (α, \tilde{C}) , and the two most important sufficient conditions for the present exposition are the following.

Condition I C is a covariance matrix and $\alpha \in (0, \frac{2}{m-1}) \cup \{\frac{2}{m-1}, \frac{2}{m-2}, \dots, 1, 2\}$.

Condition II \tilde{C} has non-negative entries and $\|\tilde{C}\| < 1$.

Condition I is a minor extension of the corresponding result in Vere-Jones (1997), and it can be found in e.g. Shirai (2007). It is related to the double stochastic construction of the α -permanental random field described in Section 4.1, which is particularly simple when $\alpha = 2/k$ for $k \in \mathbb{N}$. The sufficiency of Condition II is an immediate consequence of (17) in Section 3.3, where the density of the α -permanental random field is expressed using α -determinants of \tilde{C} . Note that α can be any positive number under Condition II.

One important necessary condition C must satisfy is

$$C(s, s) \geq 0 \quad \text{for all } s \in S. \quad (6)$$

This follows later from equation (8).

Finally, a useful expansion for $\|z_s\| \leq 1$, $s \in S$, is

$$-\log |I - Z\tilde{C}| = \sum_{n=1}^{\infty} \text{tr} \left\{ \left(Z\tilde{C} \right)^n \right\} / n \quad \text{if } \|\tilde{C}\| < 1. \quad (7)$$

See e.g. Goulden and Jackson (1983).

3 Properties of α -permanental random fields

In accordance with Shirai (2007) we define the α -determinant of an $n \times n$ matrix A with entries $A_{i,j}$ as

$$\det_{\alpha} A = \sum_{\sigma \in \mathcal{S}_n} \alpha^{n-c(\sigma)} A_{1,\sigma(1)} A_{2,\sigma(2)} \cdots A_{n,\sigma(n)}$$

where \mathcal{S}_n is the set of all permutations of $1, \dots, n$, and $c(\sigma)$ denotes the number of cycles in σ . We obtain the usual permanent if $\alpha = 1$, and if we allow $\alpha < 0$ the usual determinant $|A|$ arises in the special case $\alpha = -1$ (Minc, 1978). Note that the α -determinant is closely related to the α -permanent $|A|_{\alpha} = \alpha^n \det_{\alpha} A$ studied in Vere-Jones (1988, 1997), but $|A|_{-1} = (-1)^n |A|$ is not the determinant if n is odd.

When studying α -permanental random fields we will need various matrices formed from C and \tilde{C} . We introduce these for C in the following, while the analogous definitions for \tilde{C} simply are obtained by replacing C with \tilde{C} . For any multi-set $T = \{t_1, \dots, t_n\}$, $t_i \in S$ we let C_T denote the $n \times n$ matrix with (i, j) 'th entry $C(t_i, t_j)$. If T is of the special form

$$T = \{\underbrace{s_1, \dots, s_1}_{n_{s_1}}, \dots, \underbrace{s_i, \dots, s_i}_{n_{s_i}}, \dots, \underbrace{s_m, \dots, s_m}_{n_{s_m}}\},$$

for non-negative integers $\mathbf{n} = (n_s; s \in S)$ with $n_{\star} = \sum_{s \in S} n_s > 0$ we also write $C_T = C[\mathbf{n}]$, and we define $\det_{\alpha} C[\mathbf{0}] = 1$.

In general the computation of the permanent of a matrix is #P-complete (Valiant, 1979), which also appears to hold for the α -determinant in general when $\alpha \neq -1$. However, in Kou and McCullagh (2008) an algorithm for approximating the α -determinant for $\alpha > 0$ is given, which may help overcome the difficulties of calculating the α -determinant in applied work.

3.1 Relation to the negative binomial distribution

Let $\mathbf{N} \sim \text{per}(\alpha, C)$. From the form of (1) it is clear that for any $S' \subset S$ the subfield $\mathbf{N}_{S'} = (N_s; s \in S')$ is also a α -permanental random field; $\mathbf{N}_{S'} \sim \text{per}(\alpha, C_{S'})$. Particularly, the probability generating functions of the one dimensional marginals N_s , $s \in S$ are of the form $(1 + \alpha(1-z)C(s, s))^{-1/\alpha}$. Hence, if $b^-(\kappa, \pi)$ denotes the negative binomial distribution with parameters $\kappa > 0$ and $0 \leq \pi < 1$, and probability density function

$$\frac{\Gamma(n + \kappa)}{n! \Gamma(\kappa)} \pi^n (1 - \pi)^\kappa, \quad n = 0, 1, \dots,$$

we see that

$$N_s \sim b^- \left(\frac{1}{\alpha}, \frac{\alpha C(s, s)}{1 + \alpha C(s, s)} \right). \quad (8)$$

Consider the sum $N_\star = \sum_{s \in S} N_s$. By (1), the probability generating function of N_\star is

$$\varphi_\star(z) = |I + \alpha(1-z)C|^{-1/\alpha}. \quad (9)$$

Rewriting in terms of the eigenvalues of C , (9) yields

$$\begin{aligned} \varphi_\star(z) &= \prod_{i: \lambda_i \in \mathbb{R}} (1 + \alpha(1-z)\lambda_i)^{-1/\alpha} \\ &\times \prod_{i: \lambda_i \notin \mathbb{R}} (1 + 2\alpha(1-z)\text{Re}(\lambda_i) + \alpha^2(1-z)^2 \|\lambda_i\|^2)^{-1/(2\alpha)}. \end{aligned} \quad (10)$$

Hence, if $1/\alpha$ is an integer, the distribution of N_\star is of matrix geometrical form, see Asmussen and O'Connell (1998) and the references therein. If C only has real eigenvalues $\lambda_i \geq 0$, $i = 1, \dots, m$, then (10) implies that

$$N_\star \sim b^- \left(\frac{1}{\alpha}, \frac{\alpha \lambda_1}{1 + \alpha \lambda_1} \right) \star \dots \star b^- \left(\frac{1}{\alpha}, \frac{\alpha \lambda_m}{1 + \alpha \lambda_m} \right). \quad (11)$$

A well-known property for ‘zero-states’ of the negative binomial distribution can be generalized as follows concerning the probability

$$\varphi_{\star}(0) = \mathbb{P}(N_s = 0 \text{ for all } s \in S).$$

From (10) follows that

$$\frac{d}{d\alpha} \log \varphi_{\star}(0) = \frac{2m_1 + m_2}{2\alpha^2} - \frac{1}{2} \sum_{i: \lambda_i \notin \mathbb{R}} \|\lambda_i\|^2$$

where m_1 respective m_2 denote the number of real respective non-real eigenvalues λ_i , $i = 1, \dots, m$. Thus, if C has only real eigenvalues, $\varphi_{\star}(0)$ is an increasing function of α , and $\varphi_{\star}(0) \rightarrow 1$ for $\alpha \rightarrow \infty$.

3.2 Moments

For non-negative integers a and b , let $a^{(0)} = 1$, and $a^{(b)} = a!/(a-b)! = a(a-1) \cdots (a-b+1)$ if $a \geq b > 0$. The factorial moments are given by

$$\mathbb{E} \prod_{s \in S} N_s^{(n_s)} = \det_{\alpha} C[\mathbf{n}] \quad (12)$$

for non-negative integers $(n_s; s \in S)$. This can be obtained by expanding out the powers of $(z_s - 1)$ in (1), cf. Vere-Jones (1997) and Shirai and Takahashi (2003a). Note that (12) implies that (α, C) is such that $\det_{\alpha} C[\mathbf{n}] \geq 0$ for all non-negative integers $(n_s; s \in S)$.

In general, only the lower dimensional moments are computationally tractable. The first and second order moments are given by

$$\mathbb{E} N_s = C(s, s), \quad \text{Var} N_s = C(s, s) + \alpha C(s, s)^2, \quad \text{Cov}(N_s, N_t) = \alpha C(s, t) C(t, s), \quad \text{if } s \neq t. \quad (13)$$

By (13) it is clear that

$$N_s = 0 \text{ (almost surely)} \quad \text{if and only if} \quad C(s, s) = 0. \quad (14)$$

If $C(s, s) > 0$, we obtain from (13) the well-known property of the negative binomial distribution that N_s is over-dispersed. Moreover, (13) implies that $\text{Cov}(N_s, N_t) \geq 0$, cf. Vere-Jones (1997). Note that if C is symmetric and non-negative, there is a one-to-one correspondence between (α, C) and the moments given by (13).

If C is a covariance function, consider its correlation function

$$R(s, t) = C(s, t) / [C(s, s)C(t, t)]^{1/2}, \quad s, t \in S \quad (15)$$

where we take $R(s, t) = 0$ if $C(s, s) = 0$ or $C(t, t) = 0$. Then by (13), the correlation between N_s and N_t is

$$\text{Corr}(N_s, N_t) = \alpha R(s, t)^2 \left[\frac{C(s, s)C(t, t)}{(1 + \alpha C(s, s))(1 + \alpha C(t, t))} \right]^{1/2}, \quad s, t \in S. \quad (16)$$

The right hand side in (16) is an increasing function of α , and it tends to $R(s, t)^2$ as $\alpha \rightarrow \infty$.

3.3 Probability density function

The probability density function of an α -permanental random field can be expressed using α -determinants of \tilde{C} as follows, see Vere-Jones (1997). For any non-negative integers $\mathbf{n} = (n_s; s \in S)$ with $n_\star = \sum_{s \in S} n_s$,

$$\text{P}(\mathbf{N} = \mathbf{n}) = |I - \tilde{C}|^{1/\alpha} \alpha^{-n_\star} \det_\alpha \tilde{C}[\mathbf{n}] / \prod_{s \in S} n_s!. \quad (17)$$

This can be obtained by expanding out the powers of z_s in (3).

As described in Section 3.1 the marginal distribution of any N_s and possibly also of the ‘margin’ N_\star are related to the negative binomial distribution. However, even the joint distribution of two random variables N_s and N_t is in general complicated, cf. the discussion in Griffiths and Milne (1987).

3.4 Independence

Independence properties of infinite divisible α -permanental random fields have been studied in Griffiths and Milne (1987), and their results are summarized here with slight generalizations.

Suppose that $T, U \subset S$ are disjoint, non-empty, and let $S = T \cup U$. Recall that the subfields \mathbf{N}_T and \mathbf{N}_U are independent if and only if the probability generating function $\varphi(z_s; s \in S)$ of \mathbf{N} is a product of two functions, one of $(z_s; s \in T)$ and one of $(z_s; s \in U)$.

It follows immediately from (1) that \mathbf{N}_T and \mathbf{N}_U are independent

$$\text{if } C(t, u) = C(u, t) = 0 \text{ whenever } t \in T \text{ and } u \in U. \quad (18)$$

If C is symmetric, then by (13), $\text{Cov}(N_t, N_u) = \alpha C(t, u)^2$, and so \mathbf{N}_T and \mathbf{N}_U are independent

$$\text{if and only if } C(t, u) = 0 \text{ whenever } t \in T \text{ and } u \in U. \quad (19)$$

The property of C in (18)-(19) means that if we order the elements in S so that the elements of T come before those of U , then C restricted to $T \cup U$ is block-diagonal with respect to the partition given by T and U . If C is not symmetric, it is possible that $\text{Cov}(N_s, N_t) = C(t, u)C(u, t)$ is zero even if N_t and N_u are not independent, and we can not in general replace ‘if’ in (18) by ‘if and only if’.

Furthermore, we can replace C by \tilde{C} everywhere in (18)-(19). This follows by similar arguments as above but using (3). In addition, assume that the eigenvalues of \tilde{C} are bounded strictly in modulus by one, and define a directed graph $G(\tilde{C})$ with vertex set S and edges

$\langle s_i, s_j \rangle$ if $s_i \neq s_j$ and $\tilde{C}(s_i, s_j) \neq 0$. Then \mathbf{N}_T and \mathbf{N}_U are independent

if and only if every directed circuit in $G(\tilde{C})$ contains vertices of either T or U ,

but not both. (20)

This follows by combining (3) and (7), using similar arguments as in the proof of Theorem 3 in Griffiths and Milne (1987).

3.5 Thinning

Let $0 \leq \pi_s \leq 1$, $s \in S$, be given numbers, and consider a random field $\mathbf{N}^{\text{th}} = (N_s^{\text{th}}; s \in S)$ so that conditional on \mathbf{N} , the N_s^{th} are mutually independent and $N_s^{\text{th}} \sim b(N_s, \pi_s)$. We say that \mathbf{N}^{th} is obtained by an independent thinning of \mathbf{N} with retention probabilities π_s , $s \in S$.

Define

$$C_{s,t}^{\text{th}} = \sqrt{\pi_s \pi_t} C_{s,t}, \quad s, t \in S. \quad (21)$$

It follows immediately from (1) that

$$\mathbf{N}^{\text{th}} \sim \text{per}(\alpha, C^{\text{th}}). \quad (22)$$

Suppose that C is a covariance matrix. Then C^{th} given by (21) is also a covariance matrix, and \mathbf{N} and \mathbf{N}^{th} share the same correlation matrix R given by (15). By (16) $0 \leq \text{Corr}(N_s^{\text{th}}, N_t^{\text{th}}) \leq \text{Corr}(N_s, N_t)$, where $\text{Corr}(N_s^{\text{th}}, N_t^{\text{th}})$ is an increasing function of π_s and of π_t .

3.6 Convolution

By (1), for any $\alpha_1 > 0$ and $\alpha_2 > 0$,

$$\text{per}\left(\alpha_1, \frac{\alpha_2}{\alpha_1 + \alpha_2}C\right) \star \text{per}\left(\alpha_2, \frac{\alpha_1}{\alpha_1 + \alpha_2}C\right) = \text{per}\left(\left(\frac{1}{\alpha_1} + \frac{1}{\alpha_2}\right)^{-1}, C\right)$$

provided of course that the two first α -permanental random fields exist. In particular,

$$\text{per}(\alpha, C) = \text{per}(\alpha n, C/n)^{\star n}$$

for any $n \in \mathbb{N}$ such that $\text{per}(\alpha n, C/n)$ exists, where $\star n$ denotes convolution n times.

4 Stochastic constructions and simulation

In this section we discuss stochastic constructions and perfect simulation algorithms for the α -permanental random field \mathbf{N} . We call a simulation perfect if it (at least in theory, i.e. apart from the use of a random number generator) exactly follows a given target distribution. To exclude the trivial case where $N_s = 0$ for all $s \in S$, we assume that C has rank $r > 0$. Furthermore, we assume $m > 1$, since \mathbf{N} just follows a negative binomial distribution if $m = 1$.

4.1 Doubly stochastic construction

Assume that $\mathbf{G} = (G_s; s \in S)$ is a random field of non-negative real random variables with Laplace transform (or moment generating function) of the form

$$\mathbb{E} \exp\left(\sum_{s \in S} G_s z_s\right) = |I - \alpha ZC|^{-1/\alpha} \tag{23}$$

for $z_s \in [-1, 1]$, $s \in S$, where Z is the diagonal matrix with diagonal $(z_s; s \in S)$. This is a multivariate extension of the gamma distribution, where all one-dimensional marginals are gamma-distributed, but it is an open question to establish necessary and sufficient conditions on (α, C) for (23) to be a Laplace transform of some distribution on $[0, \infty)^m$, see Krishnamoorthy and Parthasarathy (1951) and Vere-Jones (1997). Suppose that \mathbf{N} conditioned on \mathbf{G} consists of mutually independent Poisson random variables N_s with mean G_s , $s \in S$. It is immediately verified that (1) is satisfied, so $\mathbf{N} \sim \text{per}(\alpha, C)$, cf. Vere-Jones (1997).

By this doubly stochastic construction, if we can generate \mathbf{G} , we can straightforwardly generate \mathbf{N} . Below two different constructions of \mathbf{G} are described.

Method I: Assume Condition I (Section 2.2) is satisfied. Generate a $m \times m$ Wishart matrix K with $2/\alpha$ degrees of freedom and mean C . If $G_{s_i} = K_{i,i}$ then \mathbf{G} has moment generating function (23). Simulation of Wishart distributed matrices is described in e.g. Johnson (1987).

Method II: Assume Condition I is satisfied and $\alpha = 2/k$ for some $k \in \mathbb{N}$. Generate independent zero-mean Gaussian random fields $\mathbf{Y}_1 = (Y_{1,s}; s \in S), \dots, \mathbf{Y}_k = (Y_{k,s}; s \in S)$ with covariance function C/k . If $G_s = Y_{1,s}^2 + \dots + Y_{k,s}^2$, $s \in S$, then \mathbf{G} has moment generating function (23). Various simulation methods for Gaussian random fields are implemented in the R package `RandomFields` by Martin Schlather. See also Schlather (1999), Lantuejoul (2002), and the references therein.

Method I corresponds to the extension given in Shirai (2007), and the simpler Method II

has also been considered in Vere-Jones (1997).

4.2 Poisson randomization

In the sequel, it seems more natural to work with \tilde{C} rather than C , where we assume that Condition II (Section 2.2) is satisfied. The assumption that $\tilde{C} \geq 0$ ensures that the right hand sides in the density expressions (24)-(25) and (27) below are non-negative. The α -permanental field \mathbf{N} can then be constructed by the following five steps of a Poisson randomization (a similar construction for spatial point processes was introduced in McCullagh and Møller (2006)).

1. For $n \in \mathbb{N}$, define a probability density function by

$$p_n(t_1, \dots, t_n) = \frac{1}{\text{tr}(\tilde{C}^n)} \prod_{i=1}^n \tilde{C}(t_i, t_{i+1}), \quad (t_1, \dots, t_n) \in S^n, \quad (24)$$

where $t_{n+1} = t_1$. Using the Schur decomposition of \tilde{C} (Bhatia, 1997), we obtain the normalizing constant $\text{tr}(\tilde{C}^n) = \sum_{i=1}^n \tilde{\lambda}_i^n$ of this density. It can be viewed as a Markov random field defined on the graph with vertices $1, \dots, n$ and edges $\langle i, i+1 \rangle, i = 1, \dots, n$, with the turn-around edge $\langle n, n+1 \rangle = \{n, 1\}$. It reduces to the ‘‘Ising model on the ring’’ if $S = \{s, t\}$ and $\tilde{C}(s, s) = \tilde{C}(t, t)$.

2. Define a random variable W with probability density function

$$p_W(n) = \frac{\text{tr}(\tilde{C}^n)}{Dn}, \quad n \in \mathbb{N}, \quad (25)$$

where

$$D = -\log |I - \tilde{C}|. \quad (26)$$

If the eigenvalues of \tilde{C} are real with $0 \leq \tilde{\lambda}_i < 1$, then $D = -\sum_{i=1}^m \log(1 - \tilde{\lambda}_i)$ and W follows a mixture of logarithmic distributions with parameters $\tilde{\lambda}_i$, $i = 1, \dots, m$, where the i 'th logarithmic distribution has weight $-\log(1 - \tilde{\lambda}_i)/D$ in the mixture distribution.

3. Consider an ordered point process (R_1, \dots, R_W) , where conditioned on $W = n$, (R_1, \dots, R_n) follows (24). Thus (R_1, \dots, R_W) takes values in the countable set $\cup_{n=1}^{\infty} S^n$, and its probability density function $p(t_1, \dots, t_n) = p_W(n)p_n(t_1, \dots, t_n)$ is

$$p(t_1, \dots, t_n) = \frac{1}{nD} \prod_{i=1}^n \tilde{C}(t_i, t_{i+1}), \quad (t_1, \dots, t_n) \in S^n, \quad n \geq 1. \quad (27)$$

Moreover, define a random field $\mathbf{M} = (M_s; s \in S)$ with $M_s = \sum_{j=1}^W \mathbb{I}[R_j = s]$. We call \mathbf{M} a cluster and each R_i , $i = 1, \dots, W$, a point of the cluster, i.e. M_s counts how many points in the cluster are equal to s .

4. Let V be a Poisson random variable with mean D/α , and conditioned on $V = n$, if $n > 0$, let $\mathbf{M}^{(1)}, \dots, \mathbf{M}^{(n)}$ be mutually independent copies of \mathbf{M} . These clusters are generated by corresponding mutually independent ordered point processes $(R_1^{(1)}, \dots, R_{W_1}^{(1)})$, $(R_1^{(2)}, \dots, R_{W_2}^{(2)})$, \dots , which are independent of V .

5. The Poisson randomization is given by the random field $\mathbf{N} = (N_s; s \in S)$ with

$$N_s = \sum_{i=1}^V M_s^{(i)}$$

counting how many points in all the V clusters are equal to s (setting $N_s = 0$ if $V = 0$).

The validity of this Poisson randomization is stated and proven below.

Proposition 1 *Let Condition II be satisfied. Then the random field \mathbf{N} given by the Poisson randomization 1.–5. has a probability generating function of the form (3), i.e. $\mathbf{N} \sim \text{per}(\alpha, C)$.*

PROOF:

The proof in McCullagh and Møller (2006) of the validation of the Poisson randomization is based on density calculations. Below we give an alternative, short, and simple proof based on the probability generating function.

Let $z_s \in [-1, 1]$, $s \in S$. By the construction of \mathbf{N} in the Poisson randomization, and by first conditioning on V , and next using that V is Poisson distributed with mean D/α , we obtain

$$\mathbb{E} \prod_{s \in S} z_s^{N_s} = \mathbb{E} \left[\left(\mathbb{E} \prod_{s \in S} z_s^{M_s} \right)^V \right] = \exp \left[\frac{D}{\alpha} \left(\mathbb{E} \prod_{s \in S} z_s^{M_s} - 1 \right) \right]. \quad (28)$$

By the construction of \mathbf{M} and (27),

$$\begin{aligned} \mathbb{E} \prod_{s \in S} z_s^{M_s} &= \sum_{n=1}^{\infty} \sum_{(t_1, \dots, t_n) \in S^n} \prod_{s \in S} z_s^{\sum_{j=1}^n \mathbb{I}[t_j=s]} p(t_1, \dots, t_n) \\ &= \frac{1}{D} \sum_{n=1}^{\infty} \sum_{(t_1, \dots, t_n) \in S^n} \frac{1}{n} \prod_{j=1}^n z_{t_j} \tilde{C}(t_j, t_{j+1}) \\ &= \frac{1}{D} (-\log |I - Z\tilde{C}|) \end{aligned} \quad (29)$$

where the last identity follows from (7). Combining (26) and (28)-(29) yields

$$\mathbb{E} \prod_{s \in S} z_s^{N_s} = \exp \left[\frac{1}{\alpha} \left(-\log |I - Z\tilde{C}| + \log |I - \tilde{C}| \right) \right] = \left(|I - \tilde{C}| / |I - Z\tilde{C}| \right)^{1/\alpha}$$

which agrees with the probability generating function (1).

Incidentally, if $C' = \alpha C$ is fixed, then $\mathbf{N}|(N_{S^*} > 0)$ can be seen to converge in distribution to \mathbf{M} as $\alpha \rightarrow \infty$, cf. McCullagh and Møller (2006).

REMARK:

The requirement of Condition II to be satisfied can be replaced by only requiring the perma-

mental random field to be infinitely divisible (which is implied by Condition II). Infinitely divisibility has been characterized by Griffiths and Milne (1987) and it is shown that it implies both $\|\tilde{C}\| < 1$ and that all cyclic products formed using \tilde{C} are non-negative which ensures the density (27) is still well-defined.

4.3 Perfect simulation of the Poisson randomization

Let the situation be as in Section 4.2. Perfect simulation of a realization from the Poisson randomization is straightforward if we know how to make a perfect simulation of a cluster as given in steps 1.-2. This can be done by first generating a realization $W = n$ from (25), and then use the following sequential simulation scheme. From (24) follows by induction that for any $n \in \mathbb{N}$,

$$p_{n-i}(t_1, \dots, t_{n-i}) = \frac{1}{\text{tr}(\tilde{C}^n)} \tilde{C}^{i+1}(t_{n-i}, t_1) \prod_{j=1}^{n-i-1} \tilde{C}(t_j, t_{j+1}), \quad i = 0, 1, \dots, n-1,$$

where we set $\prod_{j=1}^{n-i-1} \dots = 1$ if $i = n-1$. Hence, first we draw t_1 from the probability density function

$$p_1(t_1) \propto \tilde{C}^n(t_1, t_1)$$

and second, successively for $i = 2, \dots, n$, since $t_i|(t_1, \dots, t_{i-1}) \sim t_i|(t_1, t_{i-1})$, we draw t_i from the conditional probability density function

$$p_{i|1, i-1}(t_i|t_1, t_{i-1}) \propto \tilde{C}^{n-i+1}(t_i, t_1) \tilde{C}(t_{i-1}, t_i).$$

5 Examples

In this section, specific examples of α -permanental random field models are studied.

5.1 Example I

Let $C = \kappa Q$, where $\kappa > 0$ and Q is a projection of rank $r > 0$. In this special case \mathbf{N} satisfies many striking and unusual properties, and we refer therefore to it as the special α -permanental random field.

Recall that a real $m \times m$ matrix Q is a projection if $Q^2 = Q$, and it has then r unit eigenvalues and $m - r$ zero eigenvalues, where r is the rank of Q . As verified in Appendix B, Q is a (real) projection of rank r if and only if it is of the form

$$Q = U \begin{bmatrix} I_r & B \\ 0_1 & 0_2 \end{bmatrix} U^* = U_1 U_1^* + U_1 B U_2^* \quad (30)$$

for an arbitrary unitary matrix $U = [U_1 \ U_2]$ and an arbitrary complex $r \times (m - r)$ matrix B such that $U_1 B U_2^*$ is a real $m \times m$ matrix, where I_r is the $r \times r$ identity matrix, and 0_1 and 0_2 are corresponding zero-matrices. Here the columns in the matrix $(B U_2^*)^* = U_2 B^*$ are arbitrary complex vectors in the orthocomplement to the complex linear subspace given by the span of the columns in U_1 . Combining (2) and (30), it follows that

$$C \text{ and } \tilde{C} \text{ are proportional if and only if } C \text{ is proportional to a projection.} \quad (31)$$

Since C has r non-zero eigenvalues which are all equal to κ , (11) reduces to

$$N_\star \sim b^- (r/\alpha, \alpha\kappa/(1 + \alpha\kappa)).$$

Further, $\tilde{C} = (\alpha\kappa/(1 + \alpha\kappa))Q$, and we obtain from (12) and (17) that the expressions for the factorial moments and the probability density function are closely related, since

$$\mathbb{E} \prod_{s \in S} N_s^{(n_s)} = \kappa^{n_\star} \det_\alpha Q[\mathbf{n}], \quad \mathbb{P}(\mathbf{N} = \mathbf{n}) = \frac{\kappa^{n_\star} \det_\alpha Q[\mathbf{n}]}{(1 + \alpha\kappa)^{n_\star + r/\alpha} \prod_{s \in S} n_s!} \quad (32)$$

where $n_\star = \sum_{s \in S} n_s$.

If Q has non-negative entries, the procedure for perfect simulation of a cluster (Section 4.3) simplifies, since $\tilde{C}^i = (\alpha\kappa/(1+\alpha\kappa))^i Q$ for any $i \in \mathbb{N}$, and the conditional probability density functions

$$p_{i|1,i-1}(t_i|t_1, t_{i-1}) \propto Q(t_i, t_1)Q(t_{i-1}, t_i), \quad i = 2, \dots, n,$$

are of the same form.

5.2 Example II

If C has rank one it can be written on the form, $C_{i,j} = a_i b_j$, $i, j = 1, \dots, m$, for some real vectors (a_1, \dots, a_m) and (b_1, \dots, b_m) . We will assume that C is of this form with $\sum_{i=1}^m C_{i,i} > 0$. The matrix $A := (I-Z)C$ appearing in (1) has (i, j) 'th entry $(1-z_i)a_i b_j$. If A is a non-zero matrix, i.e. $z_i \neq 1$ for all $i = 1, \dots, m$, then A has rank one and eigenvalue $\sum_{i=1}^m (1-z_i)C_{i,i}$ with corresponding eigenvector $((1-z_1)a_1, \dots, (1-z_m)a_m)^\top$. Consequently, by (1),

$$\varphi(\mathbf{z}) = \left(1 + \alpha \left[\sum_{i=1}^m (1-z_i)C_{i,i} \right] \right)^{-1/\alpha}.$$

It follows that the distribution of \mathbf{N} depends only on C through the diagonal elements. Consequently, we may without loss of generality assume C to be a positive definite symmetric matrix with non-negative entries of the form $C_{i,j} = \sqrt{c_i c_j}$ for some non-zero vector $\mathbf{c} = (c_1, \dots, c_m)$, $c_i \geq 0$, $i = 1, \dots, m$. Then the only non-zero eigenvalue of C is $\kappa := \sum_{i=1}^m c_i = \sum_{i=1}^m C_{i,i}$, and it is a special α -permanental random field as discussed in Example I with $Q = \frac{1}{\kappa}C$. From (11) we have

$$N_\star \sim b^- \left(\frac{1}{\alpha}, \frac{\alpha\kappa}{1+\alpha\kappa} \right). \quad (33)$$

By differentiation of the probability generating function it is straightforward to find the probability of $\mathbf{N} = \mathbf{n}$ for any vector of non-negative integers $\mathbf{n} = (n_1, \dots, n_m)$ with $\sum_{i=1}^m n_i = n_\star$

$$p(\mathbf{n}) = \frac{\Gamma(\frac{1}{\alpha} + n_\star)}{\Gamma(\frac{1}{\alpha})} (1 + \alpha\kappa)^{-n_\star - \frac{1}{\alpha}} \prod_{i=1}^m \frac{c_i^{n_i}}{n_i!}.$$

Combining this with (33) yields

$$p(\mathbf{n}|n_\star) = n_\star! \prod_{i=1}^m \frac{1}{n_i!} \left(\frac{c_i}{\kappa}\right)^{n_i} \quad (34)$$

such that $\mathbf{N}|n_\star$ is multinomial with event probabilities $\frac{c_1}{\kappa}, \dots, \frac{c_m}{\kappa}$.

In this setup the random field is directly parameterized by the mean $(\mathbb{E}N_1, \dots, \mathbb{E}N_m) = (c_1, \dots, c_m)$, and using the fact that N_\star follows a negative binomial distribution and that $\mathbf{N}|N_\star$ is multinomial makes a two step perfect simulation scheme straightforward. The correlation between N_i and N_j is

$$\text{Corr}(N_i, N_j) = \sqrt{\frac{c_i}{1/\alpha + c_i} \frac{c_j}{1/\alpha + c_j}}$$

so sites with a large mean is more strongly correlated to all other sites than a site with a smaller mean. If \mathbf{N} is homogeneous in the sense that $c_1 = \dots = c_m = c$ the correlation between the counts at any two sites is $\text{Corr}(N_i, N_j) = \alpha c / (1 + \alpha c)$. Furthermore, as is the case for α -permanental random fields in general, correlation grows with α as well.

Figure 1 shows four realizations of such a homogeneous random field with $c = 100$ and $\alpha = 1$. The figure exemplifies how the correlation in this model effectively results in very little variation within a realization of the random field compared to the large variation between realizations. Based on 1000 simulations the average of the empirical variance within each realization was 15.4 compared to the marginal variance $\text{Var}(N_i) = 110$, $i = 1, \dots, 2500$. While this model is mathematically tractable it seems to be of less interest in applications

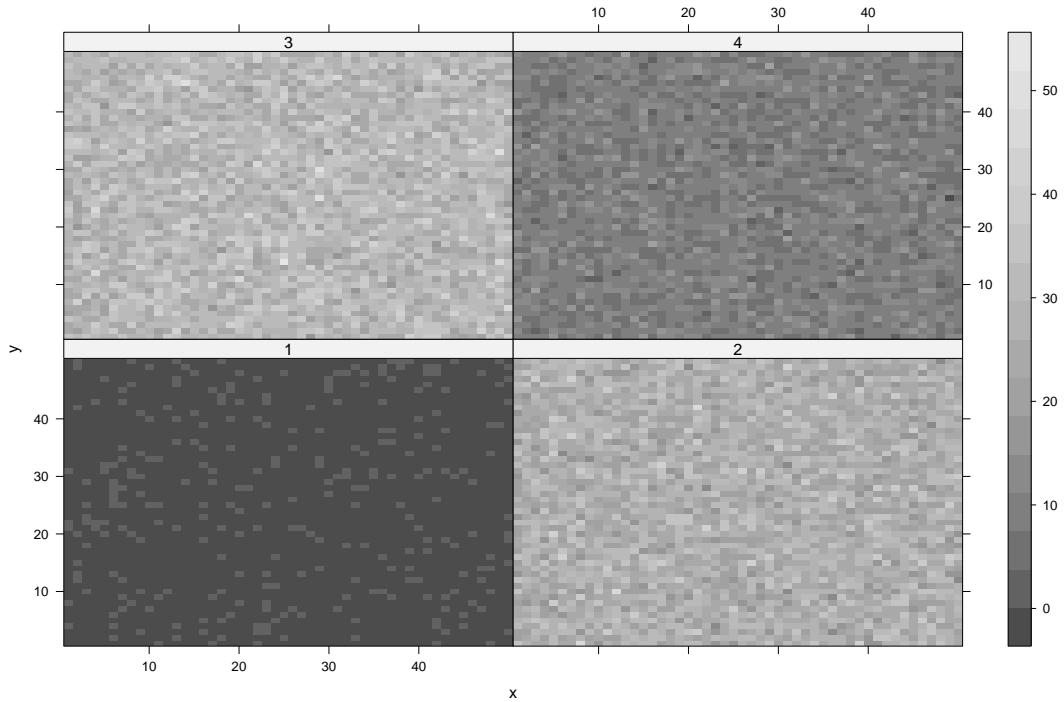


Figure 1: Four independent realizations of the random field of Example II on a 50×50 grid with $c_1 = \dots = c_{2500} = 10$ and $\alpha = 1$.

due to low flexibility, and in spatial applications the model is unaffected by usual neighborhood relations based on distances since correlation structures only depend on the mean values at any given given pair of sites.

REMARK:

In Example II it was sufficient to let C be symmetric, but this is not in general possible for an α -permanental random field where C has rank higher than one. Take e.g. $\mathbf{N} \sim \text{per}(\alpha, C)$ with C a non-symmetric matrix such that the α -permanental random field is well-defined. Then a corresponding random field parameterized by a symmetric matrix C' would have to be given by $C'_{i,j} = \sqrt{C_{i,j}C_{j,i}}$ for the covariances to be the same, but the distribution is in

general not the same using C and C' since the corresponding α -determinants (and thereby the factorial moments) differ when the rank is higher than one.

5.3 Example III

In this example, we consider a model for an α -permanental random field in the case where $S = \{s_1, \dots, s_m\}$ is a finite number of sites on the real line with $s_1 < \dots < s_m$. First a slight modification of the double stochastic construction of $\mathbf{N} = (N_s; s \in S)$ as described in Method II (Section 4.1) is considered, and we therefore require that $\alpha = 2/k$ for some $k \in \mathbb{N}$. Furthermore, for each $s \in S$, let $z(s) = (z_0(s), z_1(s), \dots, z_p(s))$ be given covariates for N_s , where we let $z_0(s) = 1$ for all $s \in S$ such that β_0 introduced below has the interpretation of an intercept on the log-scale. The random mean field $\mathbf{M} = (M_s; s \in S)$ is modeled as $M_s = \exp(\beta^\top z(s))(Y_{1,s}^2 + \dots + Y_{k,s}^2)$, where $\mathbf{Y}_1 = (Y_{1,s}; s \in S), \dots, \mathbf{Y}_k = (Y_{k,s}; s \in S)$ are independent zero-mean Gaussian random fields with the exponential covariance matrix $\text{Cov}(Y_{i,s}, Y_{i,t}) = \rho^{|s-t|}$, $0 < \rho < 1$. Suppose that \mathbf{N} conditioned on \mathbf{M} consists of mutually independent Poisson random variables N_s with mean M_s , $s \in S$. Then $\mathbf{N} \sim \text{per}(\alpha, C)$, where

$$C_{i,j} = C(s_i, s_j) = \exp\left(\beta^\top(z(s_i) + z(s_j))/2\right) \rho^{|s_i - s_j|}. \quad (35)$$

Using this construction the model is at least well-defined for $\alpha = 2/k$, $k \in \mathbb{N}$, but the following proposition extends the model to all $\alpha > 0$.

Proposition 2 *Let $S = \{s_1, \dots, s_m\}$, $s_1 < \dots < s_m$, $0 < \rho < 1$, and $\alpha > 0$. If C is given by (35) then all entries of $\tilde{C} = \alpha C(I + \alpha C)^{-1}$ are non-negative and $\text{per}(\alpha, C)$ is thus well-defined.*

PROOF:

We have $C = DBD$, where D is a diagonal matrix with $D_{i,i} = \exp(\beta^\top z(s_i)/2)$, $i = 1, \dots, m$, and B is the matrix with entries $B_{i,j} = \rho^{|s_i - s_j|}$. Using a notation as in Appendix A, B is a Green's matrix with $a_i = \rho^{-|s_i - s_1|}$ and $b_i = \rho^{|s_i - s_1|}$. Thus, if the inverse $B^{-1} = T$ exists, T is tridiagonal, and it is straightforward to verify that the matrix T given in the following is indeed the inverse of B . The diagonal elements are

$$T_{i,i} = \frac{1 - \rho^{2|s_{i+1} - s_{i-1}|}}{(1 - \rho^{2|s_{i+1} - s_i|})(1 - \rho^{2|s_i - s_{i-1}|})}, \quad i = 1, \dots, m$$

where we define $s_0 = s_{m+1} = \infty$, such that $\rho^{2|s_1 - s_0|} = \rho^{2|s_2 - s_0|} = \rho^{2|s_{m+1} - s_m|} = \rho^{2|s_{m+1} - s_{m-1}|} =$

0. The non-zero off-diagonal elements are

$$T_{i,i+1} = T_{i+1,i} = \frac{-\rho^{|s_{i+1} - s_i|}}{1 - \rho^{2|s_{i+1} - s_i|}}, \quad i = 1, \dots, m-1.$$

Now,

$$\tilde{C} = (I + (\alpha C)^{-1})^{-1} = (I + \alpha^{-1} D^{-1} B^{-1} D^{-1})^{-1} = \alpha D (\alpha D^2 + T)^{-1} D,$$

where the first equality follows by the Woodbury matrix identity (Woodbury, 1950) since C is non-singular. Clearly the matrix αD^2 is diagonal and positive definite. The sum of positive definite matrices is positive definite, so $(\alpha D^2 + T)$ is a symmetric positive definite tridiagonal matrix with non-positive off-diagonal elements. Lemma 1 in Appendix A implies that all elements of $(\alpha D^2 + T)^{-1}$ are non-negative, and the result follows.

Figure 2 is inspired by a dataset that fits into this setup (counts of clover leaves in 200 squares of size 5×5 cm along a 10 m transect line, see Augustin *et al.* (2006)), where the data can be viewed as a one-dimensional random field consisting of 200 sites on the real line with positive association expected between the counts due to clustering of clovers in

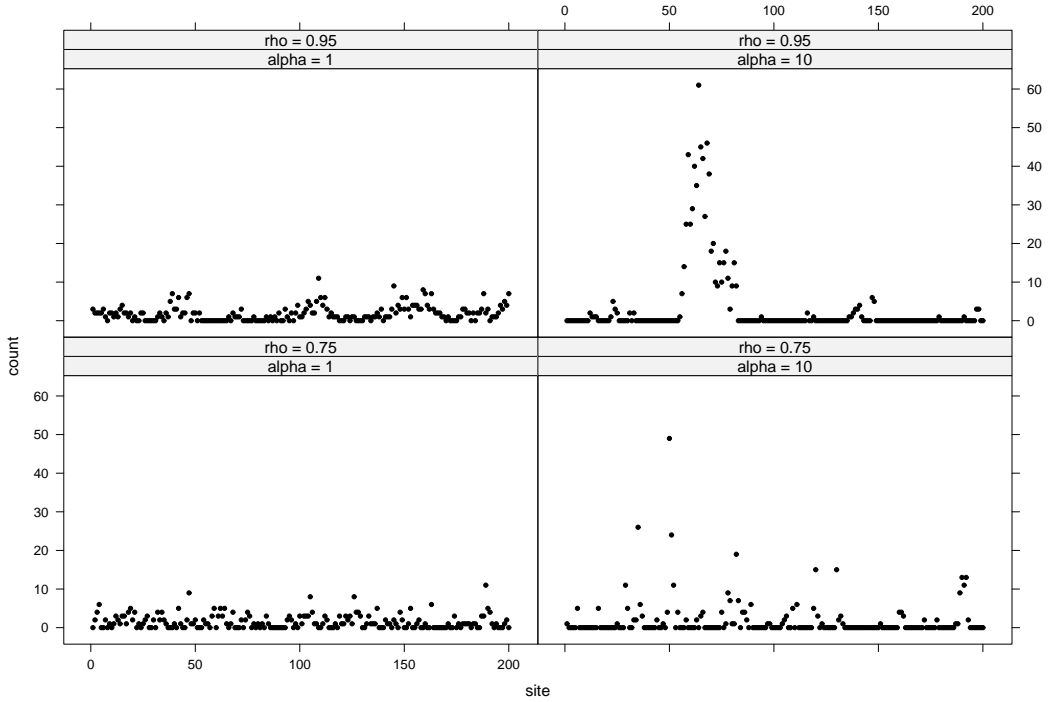


Figure 2: Realizations of the random field of Example III for different values of α and ρ .

patches. Figure 2 shows four different simulated datasets of this type using different values of α and ρ . Since no covariates are available the only other parameter in the model is β_0 , which controls the mean value $EN_1 = \dots = EN_{200} = \exp(\beta_0)$. For different values of (α, ρ) , permanent random fields were simulated using the Poisson randomization described in Section 4.2, where $\beta_0 = \log(1.28)$ is fixed so that the random fields have the same mean as the data from Augustin *et al.* (2006). Table 5.3 summarizes some characteristics for each of the simulated models. Here the correlation between neighboring sites is straightforward to calculate, and for the real data the empirical estimate is reported. Further, V is the number of clusters in a simulation, and from both its mean and its four simulated values it is clear that realizations of V tend to be higher for smaller values of α and ρ . On the other hand, realizations of W , which denotes the size of a cluster, tends to be larger for larger

values of α and ρ . This gives an intuitive understanding of how the dependence structure is created in the Poisson randomization: Large values of α lead to a small number of very large clusters, and large values of ρ makes the correlation within the cluster high, such that a few close sites are sampled many times in a cluster. Simulations 1 and 2 ($\alpha = 1$) were also done

Simulation	1	2	3	4	Real data
(α, ρ)	(1, 0.75)	(1, 0.95)	(10, 0.75)	(10, 0.95)	-
$E(N_s)$	1.28	1.28	1.28	1.28	1.28
$\text{Corr}(N_{s_i}, N_{s_{i+1}})$	0.316	0.507	0.522	0.837	0.508
$E(V)$	119	63	39	21	-
$P(W = 1)$	0.627	0.563	0.408	0.475	-
$P(W \leq 2)$	0.793	0.706	0.575	0.623	-
$P(W \leq 10)$	0.980	0.919	0.869	0.849	-
$P(W \leq 100)$	1.000	0.999	0.994	0.975	-
V	130	62	45	20	-
\bar{W}	2.29	5.85	8.18	34.9	-

Table 1: Parameter values and characteristics of the four simulated random fields considered in Example III. The bottom two rows are observed quantities for the specific simulation whereas the other values are calculated theoretically. The right most column shows the empirical mean and lag 1 autocorrelation of one of the real data sets from Augustin *et al.* (2006).

using the double stochastic construction of Section 4.1 to compare simulation time of the two algorithms. In the Poisson randomization the most computer intensive part is calculating

all the necessary powers of \tilde{C} used both to simulate the cluster length W and in the perfect simulation of a cluster, cf. Sections 4.2-4.3. After this initialization repeated simulations of the random field are faster and 1,000 simulations only take about 20 times longer to generate as the first simulation alone. It is however much faster to use the double stochastic scheme, which for 1,000 simulations took only 1/30 of the corresponding simulation time for the Poisson randomization.

6 Extensions

6.1 Extension to infinite random fields

In the following we consider extensions of the α -permanental random field to $S = \cup_{i=1}^{\infty} S_i$ for finite $S_1 \subseteq S_2 \subseteq \dots$. Suppose that $\alpha > 0$ and $C : S \times S \rightarrow \mathbb{R}$ are such that $\mathbf{N}_{S_i} \sim \text{per}(\alpha, C_{S_i})$ for any $i = 1, 2, \dots$, where C_{S_i} denotes the restriction of C to $S_i \times S_i$. Then $\mathbf{N}_{S_1}, \mathbf{N}_{S_2}, \dots$ form a consistent family of finite dimensional random fields, so the extension to all of S , $\mathbf{N} = \mathbf{N}_S$, is thus well-defined, and we still write $N \sim \text{per}(\alpha, C)$.

Conditions and properties of the α -permanental field generalizes easily to this case. For example, in place of Condition II (Section 2.2) we may now require that for every integer $j > 0$ exists an integer $i \geq j$ such that \tilde{C}_{S_i} has non-negative entries and $\|\tilde{C}_{S_i}\| < 1$. Then \mathbf{N} exists for any $\alpha > 0$.

6.1.1 Stationarity and inhomogeneity

Consider the special case where $S = \mathbb{Z}^d$ is the d -dimensional integer lattice. We say that \mathbf{N} is stationary if \mathbf{N} and $(N_{s+t}; s \in S)$ are identically distributed for all $t \in \mathbb{Z}^d$, and that C is

stationary if $C(s + u, t + u) = C(s, t)$ for all $s, t, u \in \mathbb{Z}^d$. It follows immediately from (1) that stationarity of \mathbf{N} is equivalent to stationarity of C .

Suppose that C_T is of rank at most one whenever $T \subset S$ is finite. Considering the extension of Example II to the case where S is infinite, we see that \mathbf{N} is stationary if and only if $C(s, t) = c$ for all $s, t \in S$, where $c \geq 0$.

Inspiration for a general method to model an inhomogeneous α -permanental random field on basis of a stationary one is found by revisiting Example III. This model has a possibly inhomogeneous mean $\mu = (\mu_s; s \in S)$ based on covariates, and an alternative construction of the model is as an independent thinning of a permanental random field with constant mean $\tilde{\mu}_0$ for all $s \in S$, provided $\tilde{\mu}_0 \geq \sup\{\mu_s; s \in S\}$. The retention probabilities would then be $\pi_s = \mu_s/\tilde{\mu}_0$, $s \in S$.

6.2 Determinantal random fields

If $\alpha < 0$ is allowed in Definition 1, a new class of random fields called α -determinantal random fields emerges. These random fields are well-studied in Vere-Jones (1997), and they share many of the properties of α -permanental random fields as well as there are differences. For example, $1/\alpha$ needs to be an integer. The formulae for the moments and the probability density are still given by (12) and (17), but due to the sign change of α , the α -determinantal random fields exhibit negative correlations and under dispersion. Furthermore, they are multivariate extensions of the binomial distribution instead of the negative binomial distribution. The simulation of an α -determinantal random field can be done by a kind of stochastic Gram-Schmidt orthogonalization as described by Hough *et al.* (2006).

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A Green’s matrices and tridiagonal matrices

We will need some results on Green’s matrices and tridiagonal matrices (sometimes called Jacobi matrices). The results presented here are either from Karlin (1968) or direct consequences of results herein.

A Green’s matrix is a symmetric $n \times n$ matrix G with $G_{ij} = a_{\min(i,j)} b_{\max(i,j)}$ for some $a_1, \dots, a_n, b_1, \dots, b_n \in \mathbb{R}$. If G is invertible, then it is a Green’s matrix if and only if the inverse $T = G^{-1}$ is symmetric and tridiagonal.

For any $n \times n$ matrix A and any $\{i_1, \dots, i_m\} \subseteq \{1, \dots, n\}$ we introduce the minor of A , $m_A(i_1, \dots, i_m)$, as the determinant of the matrix obtained from A by deleting all other rows and columns than i_1, \dots, i_m . If a symmetric tridiagonal matrix T is positive definite, any minor of T is positive.

The (i, j) ’th element of the inverse T^{-1} is given as the following (due to symmetry we only need to specify the elements with $i \leq j$). If $i = j$, then

$$T_{i,i}^{-1} = \frac{1}{|T|} m_T(1, \dots, i-1, i+1, \dots, n).$$

If $i < j$, then

$$T_{i,j}^{-1} = \frac{(-1)^{j+i}}{|T|} m_T(1, \dots, i-1) T_{i,i+1} T_{i+1,i+2} \cdots T_{j-1,j} m_T(j+1, \dots, n).$$

Consequently, a sufficient condition for all elements of T^{-1} to be non-negative is that the off-diagonal elements are non-positive and T is positive definite. This result is summarized in the following lemma.

Lemma 1 *Let T be a symmetric tridiagonal matrix. If T is positive definite and $T_{i,j} \leq 0$ for all $i \neq j$, then $T_{i,j}^{-1} \geq 0$ for all i, j .*

B Schur decomposition of a projection

This appendix verifies that a real $m \times m$ matrix Q of rank r is a projection if and only if it is of the form (30).

Assume that Q is a projection. Combining this assumption with the Schur decomposition (Bhatia, 1997), Q is seen to be of the form $Q = U\Delta\bar{U}$ for some unitary matrix U and some lower triangular matrix Δ with the first r diagonal elements equal to one and the remaining $m - r$ diagonal elements equal to zero, and so that $\Delta^2 = \Delta$. Writing Δ on the block form

$$\Delta = \begin{bmatrix} A & B \\ 0_1 & E \end{bmatrix}$$

with similar dimensions of the four matrices as those in (30), it follows from $\Delta^2 = \Delta$ that $A = A^2$, $B = AB + BE$, and $E = E^2$. Thus the first identity in (30) is equivalent to that $A = I_r$ and $E = 0_2$. Since $A = A^2$ is upper triangular with all diagonal elements equal to one, we obtain first by considering the elements $a_{i,i+1}$ above the diagonal that $a_{i,i+1} = 2a_{i,i+1}$, i.e. $a_{i,i+1} = 0$, and second by considering the elements $a_{i,i+2}$ twice above the diagonal that

$a_{i,i+2} = a_{i,i+2} + a_{i,i+1}a_{i+1,i+2} + a_{i,i+2} = 2a_{i,i+2}$, i.e. $a_{i,i+2} = 0$, and in a similar way by induction it follows that $A = I_r$. Since $E = E^2$ is strictly upper triangular, we obtain first that the elements $e_{i,i+1}$ above the diagonal are zero, and second that the elements $e_{i,i+2}$ twice above the diagonal satisfy $e_{i,i+2} = e_{i,i+1}e_{i+1,i+2} = 0$, and so on, i.e. $E = 0_2$. Hence the first identity in (30) is obtained, while the other identity immediately follows.

On the other hand, if (30) holds, then it follows immediately that Q is a projection of rank r .

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