Perfect simulation and moment properties for the Matérn Type III Process

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Abstract The Matérn type III hard core point process (shortly Matérn III process) is a less well-known but for many applications more appealing or realistic model than the Matérn type I and II hard core point processes. This paper focuses on the stationary (and hence infinite) Matérn III process from a probabilistic and a stochastic geometry perspective. Briefly, given a hard core parameter $R > 0$, the Matérn III process is obtained by a dependent thinning from a spatio-temporal Poisson process on $\mathbb{R}^d \times [0, 1]$ with intensity $\lambda > 0$, where a Poisson point becomes a Matérn III point if the ball of radius R centered at the point does not contain an earlier Matérn III point. Using a construction of Matérn III that creates various 'generations' of points, a perfect simulation algorithm for the infinite Matérn III process within a bounded region is developed. It is shown that the log expected number of points that must be examined is bounded above by a linear function which is easily calculated. This result is quite general, which is illustrated by an extension of the basic Matérn III process to allow random radii or more generally to replace balls with random sets, and also to allow spatial inhomogeneity. The perfect simulation algorithm is used to provide Monte Carlo estimates of the packing density of Matérn III, which can be much higher than for Matérn I or II, and increases to the jamming limit of the random sequential adsorption model as $\lambda \to \infty$.

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1 Introduction

Bertil Matérn introduced in his seminal D. Sc. thesis work (Matérn, 1960) several important spatial models, including what are now known as the Matérn hard core point processes of types I and II (hereafter just called Matérn I and II), see Matérn (1986, pp. 47–49) and e.g. Stoyan, Kendall, and Mecke (1995, p. 121). Given a hard core parameter $R > 0$ and a stationary Poisson point process in $\mathbb{R}^d$ with intensity $\lambda > 0$, which (following Matérn) we call the primary process, Matérn I is the secondary point process obtained by retaining every primary point which is not within distance R from another primary point. Upon assigning to the primary points independent time marks chosen uniformly from the interval $[0, 1]$, Matérn II is the secondary point process obtained by retaining every primary point z which is not within distance R from another primary point with a lower (or 'earlier') time mark. Matérn briefly mentioned a third type of hard core process, where instead every primary point z is retained if no earlier *secondary* point is within distance R (Matérn, 1986, page 48); the details are given in Section 2.

This paper deals with this less well-known but for many applications more appealing or realistic hard core point process model which we refer to as the stationary Matérn's hard core process of type III or shortly Matérn III. Although Matérn discusses the model no further after noting that 'even an attempt to find the [packing density] tends to rather formidable mathematics', the Matérn III process on spaces such as $\mathbb{R}^d$ can be constructed and simulated (Penrose, 2001). Likelihood-based inference for a version of the Matérn III process on bounded sets is considered by Huber and Wolpert (2009), whereas the focus in the present paper is on the stationary (and hence infinite) Matérn III process from a probabilistic and a stochastic geometry perspective. We shall also consider various extensions of the Matérn III process.

As the primary intensity $\lambda \to \infty$, the Matérn III model converges to the 'jamming limit' of the random sequential adsorption (RSA) model long used by physicists and chemists studying the irreversible binding of proteins to surfaces. In its most common form this model constructs a hard core process as a sequence of points, each drawn within some bounded region $S \subset \mathbb{R}^2$ from

the uniform distribution on the complement of the unions of disks of radius R centered at each of the previously-drawn points. When this union (whose connnected components are called 'cavities') is empty, the jamming limit has been reached and the process halts. Variations include using replacing the disks with squares or other convex shapes, constructing the process in $\mathbb{R}^d$ rather than the plane, employing independent random radii R_i, stopping after a specified number of points have been drawn, stopping after a specified number of attempts have been made, *etc.* For more details and some of the historical development, see Döge (2001); Feder (1980); Finegold and Donnell (1979); Pálasti (1960); Schaaf, Voegel, and Senger (1998); Solomon (1967); Tanemura (1979).

In this paper, we present a construction of Matérn III that creates various 'generations' of points. This point of view is inspired from our simulation algorithm for the process rather than from the relationship to RSA. Section 2 presents this construction in a form similar to that found in Stoyan and Schlather (2000), but in greater detail.

Section 3 then presents the basic simulation algorithm, which is *perfect* in the sense of Propp and Wilson (1996) in that it has a random running time but returns samples drawn exactly from the desired distribution. This method was derived independently from but is similar to an algorithm implicitly given in Penrose (2001). Later in the section an improvement to the basic method is given that drastically speeds up the algorithm.

Next comes an analysis of the running time of the algorithm. In Penrose (2001) and Schreiber, Penrose, and Yukich (2007) are shown that the chance that the presence of a particular point in the process affects another point declines exponentially in the distance between them. Section 3.2 shows that the expected number of points that must be examined in order to determine whether or not to include as a secondary is bounded above by a simple function of an easily calculated parameter of the process. This result is quite general, which we illustrate by an extension of the basic Matérn III process to allow random radii or more generally to replace balls with random sets, and also to allow spatial inhomogeneity.

While first and second order moment properties can easily be derived for Matérn I and II (Matérn, 1986, page 48), no closed form expressions are available for Matérn III (Matérn, 1986, page 49). On the other hand, the likelihood function for a finite version of the marked Matérn III process can be derived in closed form (Huber and Wolpert, 2009), while this seems to be impossible for Matérn I and II. As demonstrated in this paper, although

it is harder to simulate from Matérn III than from Matérn I or II, it is still feasible to make perfect simulations and hence to study the properties of Matérn III experimentally. Section 4 provides Monte Carlo estimates of the packing density of Matérn III, which can be much higher than for Matérn I or II, and increases to the jamming limit of RSA as $\lambda \to \infty$.

2 Dependent thinning constructions

In this section, a construction for the Matérn III process is given that utilizes a generation approach whereby points are removed from a dominating process or added to the Matérn III process at each generation. This is similar to an approach described in Stoyan and Schlather (2000) that was suggested by the first author.

We shall only consider point processes expressible as locally-finite subsets of $\mathbb{R}^d$ or $\mathbb{R}^d \times [0,1]$. As described in detail below, for a given hard core parameter $R > 0$, the stationary Matérn I–III processes denoted $X_{\text{I}}, X_{\text{II}}, X_{\text{III}}$, respectively, can all be constructed by dependent thinnings from a Poisson point process Y on $\mathbb{R}^d \times [0,1]$ with intensity $\lambda > 0$. In Matérn's terminology, Y is the primary process, and $X_{\text{I}}, X_{\text{II}}, X_{\text{III}}$ the secondary processes. When we later write "by stationarity", we have in mind that the distribution of Y is invariant under translations in $\mathbb{R}^d$.

Often it is useful to view $Y = \{(z_1, t_1), (z_2, t_2), \ldots\}$ as a marked Poisson process, where the points $Z = \{z_1, z_2, \ldots\}$ constitute a stationary Poisson point process on $\mathbb{R}^d$ of intensity λ, and the marks $\{t_1, t_2, \ldots\}$ are independent uniformly distributed on $[0,1]$ and independent of Z. We shall refer to t_i as the *time* associated with point z_i. It turns out that an equivalent marked Poisson process to Y, with i.i.d. t_i following an arbitrary continuous distribution on $\mathbb{R}$, will lead to the same definitions of Matérn I–III as below, since the times then will have no ties (with probability one). It is also useful to view Y as a spatio-temporal point process, where we say that z_i is older than z_j (or z_j is younger than z_i) if $t_i < t_j$.

We say that z_i and z_j are (R-close) neighbours if their Euclidean distance satisfies $0 < \|z_i - z_j\| \leq R$, in which case (z_i, t_i) and (z_j, t_j) are also said to be neighbours. For any subprocesses $U \subseteq Z$ and $V \subseteq Y$ and points $z_i \in U$

and $(z_i, t_i) \in V$, call

$$\partial(z_i, U) := \{z_j \in U : 0 < \|z_i - z_j\| \leq R\}$$

the *neighbours* of z_i within U, and

$$\partial_<\big((z_i, t_i), V\big) := \{(z_j, t_j) \in V : \|z_i - z_j\| \leq R,\, t_j < t_i\}$$

the *older neighbours* of (z_i, t_i) within V.

Let $B_R(z)$ denote the closed ball in $\mathbb{R}^d$ with centre z and radius R. The random graph with vertex set Z and edges connecting any two neighbouring points z_i, z_j corresponds to the Poisson process of balls $B_{R/2}(z_i)$, $z_i \in Z$, where intersecting balls are neighbours. Restricting this graph to any subprocess $Z' \subseteq Z$ and considering the corresponding marked subprocess $Y' = \{(z_i, t_i) : z_i \in Z'\}$, we refer to the subprocesses of Z' given by the maximal connected components of the subgraph with vertex set Z' as the Z'-*clusters*, and also to the corresponding subprocesses of Y' as the Y'-*clusters*. For $d \geq 2$, we have continuum percolation (Meester and Roy, 1996), since there exists a critical value $\lambda_c > 0$, such that for $\lambda > \lambda_c$ there is a positive probability that an infinite cluster exists, while for $\lambda < \lambda_c$ almost surely no infinite cluster exists. The critical value is not known precisely in general. For $d = 2$ and $R = 2$, we have $0.174 < \lambda_c < 0.843$ (Meester and Roy, 1996, Theorem 3.10).

For Matérn I, a primary point $z_i \in Z$ is retained as a secondary point if and only if z_i has no neighbours in Z. Thus the time t_i plays no role, and

$$X_{\text{I}} = \{z_i \in Z : \partial(z_i, Z) = \emptyset\}$$

is the set of isolated Z-clusters (those with only one member).

For Matérn II, a primary point $z_i \in Z$ is retained as a secondary point if and only if the corresponding marked point (z_i, t_i) has no older neighbours, so

$$X_{\text{II}} = \{z_i \in Z : \partial_<\big((z_i, t_i), Y\big) = \emptyset\}.$$

Each Z-cluster contributes to X_{II} its locally oldest members, *i.e.*, those with no older neighbours.

Matérn's definition of his third type of hard core point process is that a primary point $z_i \in Z$ is retained as a secondary point if and only if z_i is not an R-close neighbour to an older retained secondary point z_j (*i.e.*, $t_j < t_i$). Thus, while in Matérn II a point $z_i \in Z$ will always be thinned by an older

neighbour $z_j \in Z \cap B_R(z_i)$, in Matérn III it will not be thinned by that z_j if z_j was already thinned by a yet earlier point.

To make this spatio-temporal definition more clear, consider the following iterative construction, which is illustrated in Figures 1–3. Begin with $Y^{(1)} := Y$, a Poisson point process on $\mathbb{R}^d \times [0,1]$ with intensity $\lambda > 0$, and, for $Z^{(1)} := Z$, $i = 1, 2, \ldots$, set

$$X^{(i)} = Y^{(i)} \setminus \bigcup_{(z,t)\in Y^{(i)}} B_R(z) \times (t, 1], \tag{1a}$$

$$Y^{(i+1)} = Y^{(i)} \setminus \bigcup_{(z,t)\in X^{(i)}} B_R(z) \times [t, 1]. \tag{1b}$$

At each stage i, $X^{(i)}$ is obtained by thinning $Y^{(i)}$ in exactly the same way as in Matérn II, that is, $X^{(i)}$ consists of the locally oldest members of the $Y^{(i)}$-clusters. As verified later in Corollary 1, with probability one, within each $Y^{(i)}$-cluster there will be at least one locally oldest member, and as exemplified in Figures 1 and 3 there may be more than one locally oldest member. Furthermore, $Y^{(i+1)}$ concists of those elements in $Y^{(i)}$ which are neither in $X^{(i)}$ or thinned by an element of $X^{(i)}$. We call $Y^{(i)}$, $X^{(i)}$, and $Y^{(i)} \setminus X^{(i)}$ the i^{th} *generation primary, secondary, and complementary processes*, respectively. Finally, the Matérn III process is

$$X_{\text{III}} = \bigcup_{i=1}^{\infty} \{z : (z,t) \in X^{(i)}\}, \tag{1c}$$

the projection of $\cup_{i=1}^{\infty} X^{(i)}$ onto $\mathbb{R}^d$. Note that the projection of $X^{(1)}$ onto $\mathbb{R}^d$ is just the Matérn II process X_{II}.

The coupling of the Matérn I–III processes is given in the following proposition and illustrated in Figure 4.

Proposition 1. *With probability one,* $X_{I} \subset X_{II} \subset X_{III} \subset Z$.

Proof. Since X_{I} is the set of isolated Z-clusters, and X_{II} is the projection of $X^{(1)}$ onto $\mathbb{R}^d$, it follows that $X_{\text{I}} \subseteq X_{\text{II}} \subseteq X_{\text{III}} \subseteq Z$. Hence, since there is a positive probability that $X^{(1)} \neq X^{(2)}$, it follows that the intensity of $X^{(1)}$ is strictly smaller than that of $X^{(2)}$, and so $X^{(1)} \subset X^{(2)}$ almost surely. In a similar way we obtain that $X^{(2)} \subset X^{(3)}$ and $X^{(3)} \subset Z$ almost surely. □

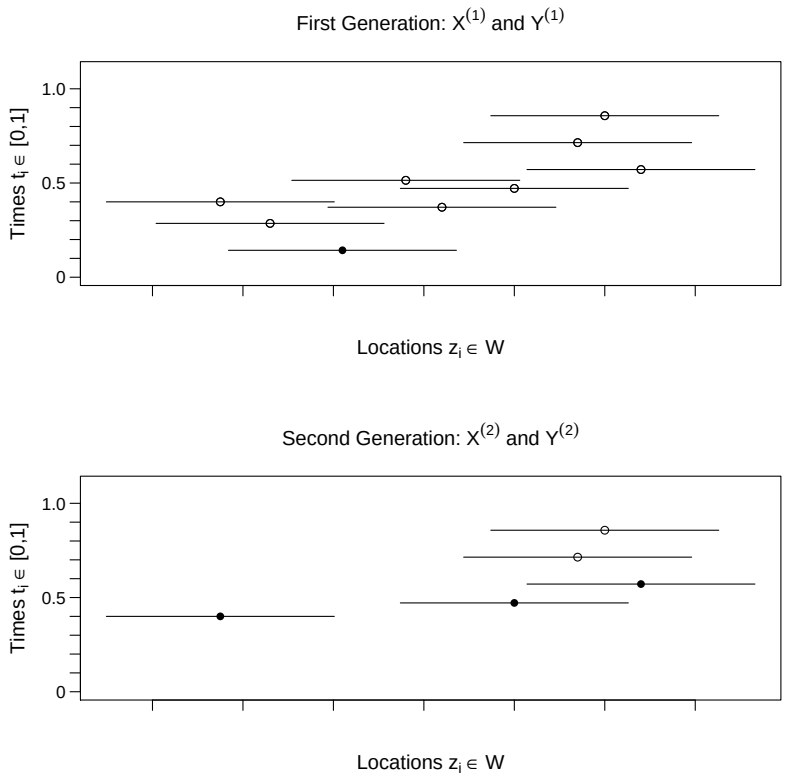

Figure 1: An illustration of a single cluster of the primary process in the one-dimensional case $d = 1$. The horizontal line segments are centered at the marked points (z_i, t_i) of the cluster and have length $2R$. The first (top panel) and second (bottom panel) generation secondary marked points are the filled circles, and the first (top panel) and second (bottom panel) generation complementary marked points are the open circles. There are no higher order generation marked points.

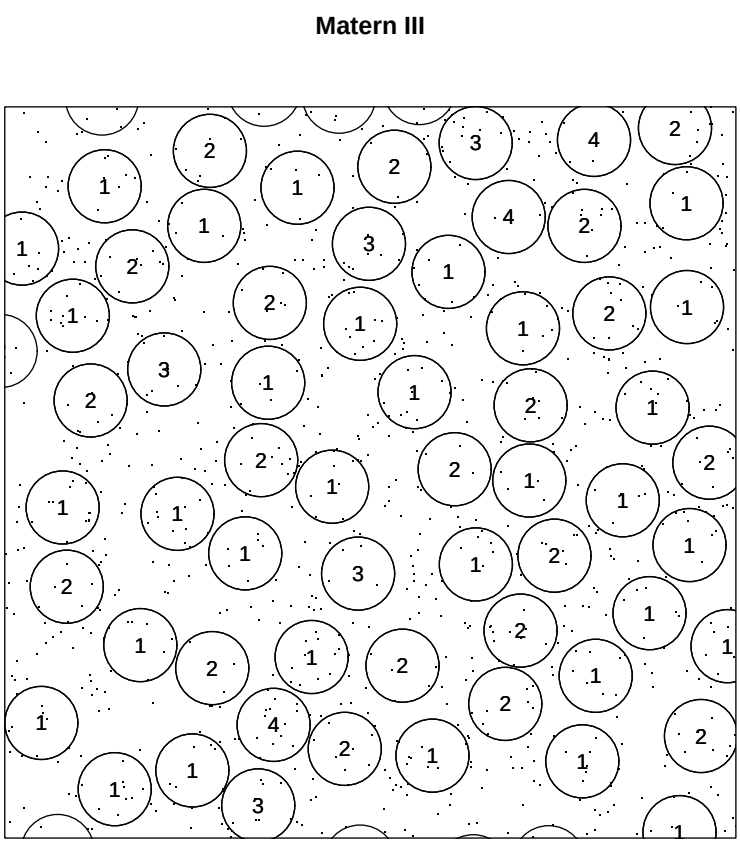

Figure 2: Perfect simulation of a Matérn III process within a rectangular region, with $\lambda = 10$ and $R = 1$. The circles are centered at the Matérn III points and are all of radius $R/2$. The integers $i = 1, 2, \ldots$ at circle centers are points of the i^{th} generation secondary process $X^{(i)}$. The dots are the primary points removed by older Matérn III points within distance R.

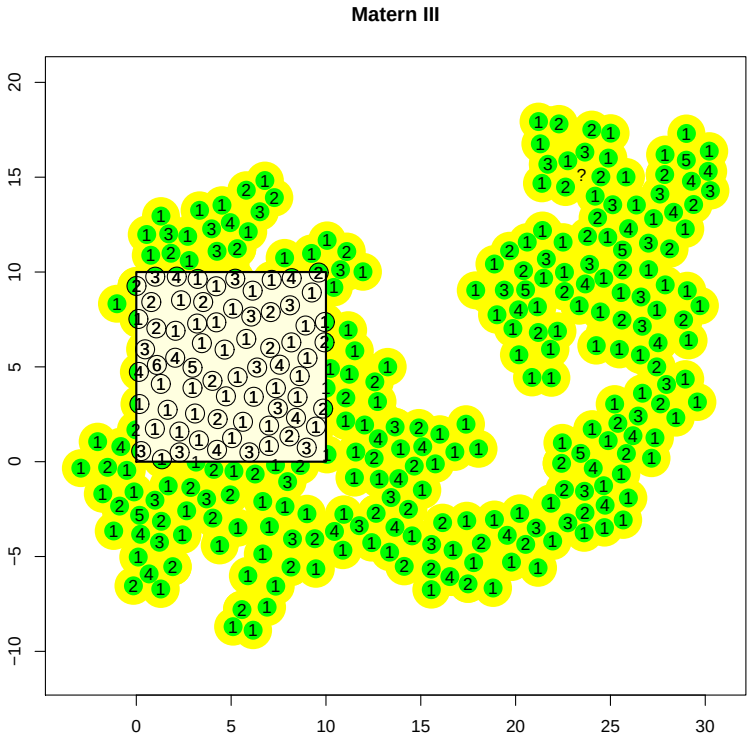

Figure 3: Perfect simulation of a Matérn III process within $W = [0, 10]^2$, with $\lambda = 100$ and $R = 1$, with 70 Matérn III points in W. The disjoint circles of radius $R/2$ are centered at the Matérn III points. The integers i are points of the i^{th} generation secondary process $X^{(i)}$ within the cluster. The numbers of secondary points within W of generation i are 38, 12, 11, 7, 1, 1 for $i = 1, \ldots, 6$, respectively. The estimated packing density (see Section 4) is $(70/100)\pi(R/2)^2 = 54.98\%$.

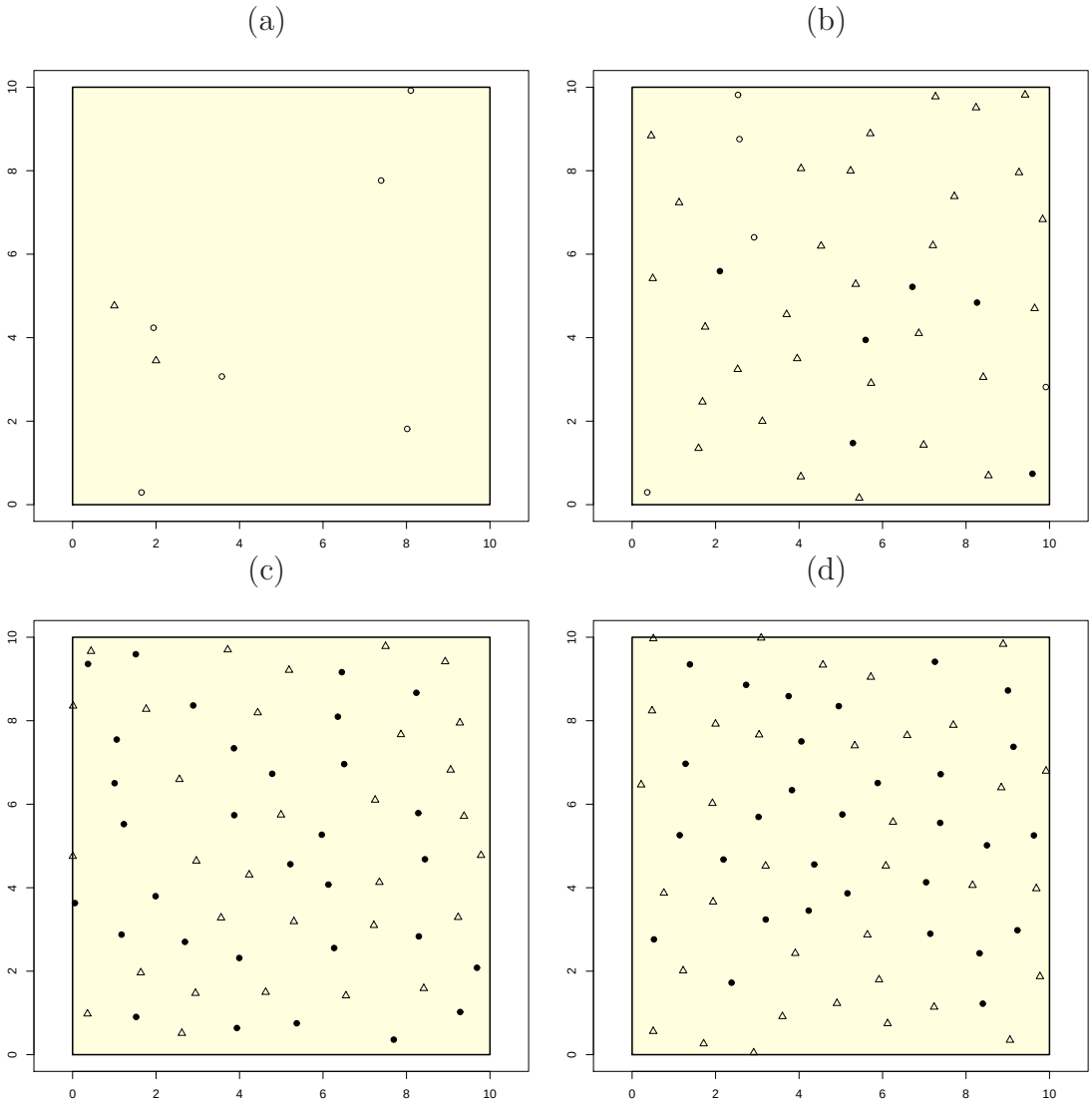

Figure 4: Planar Matérn hard core point processes at four intensities, with $R = 1$ in all cases: (a) $\lambda = 0.10$, (b) $\lambda = 1.0$, (c) $\lambda = 10.0$, (d) $\lambda = 100$. Empty circles are Matérn I–III; triangles are Matérn II–III; filled circles are Matérn III. Packing densities (see Section 4) of Matérn III are 5.5%, 31.4%, 47.9%, and 48.7%, respectively — well below the two-dimensional perfect-packing density of $\pi/\sqrt{12} = 90.7\%$, but for (b)–(d) well above the maximal Matérn II density of 25%.

3 Perfect simulation

Efficient simulation procedures are important for theoretical investigations as well as for model checking based on, *e.g.*, the reduced second moment or K-function (Ripley, 1981, §8.1). Matérn I and II can easily be simulated within a bounded region $W \subset \mathbb{R}^d$, since they do not depend on those $(z_i, t_i) \in Y$ for which the distance from z_i to W exceeds R. This section shows how to make a perfect simulation of $X_{\text{III}} \cap W$, the Matérn III process within W, without ignoring the fact that $X_{\text{III}} \cap W$ may depend on $(z_i, t_i) \in Y$ for z_i arbitrarily far away from W.

3.1 The basic algorithm

Suppose $W \subset \mathbb{R}^d$ has finite volume (Lebesgue measure). To support inference about λ and R, when only a finite point pattern $\{z_i\}_{i \in I} \subset W$ is observed and modeled by a finite version of the Matérn III process within W, Huber and Wolpert (2009) developed a perfect simulation algorithm of the latent times $\{t_i\}_{i \in I}$ and the removed marked points but without accounting for edge effects. Here we address a different problem — the perfect sampling of both the positions and times for the Matérn III process, with full accounting of the edge effects.

Our first algorithm, Algorithm 1, is implicit in early work of Penrose (2001) and was rediscovered independently by the authors. The pseudo code in Algorithm 1 below describes our perfect sampler, and Figures 5 and 6 illustrate the algorithm.

Algorithm 1 begins with setting $U = W$ and generating a primary Poisson point process Y_U of intensity $\lambda > 0$ on $U \times [0, 1]$. Clearly, Y_U is distributed as $Y \cap U \times [0, 1]$. Let Z_U denote the set of the corresponding points, which we view as $Z_U = Z \cap U$. Thus the output of the algorithm is a subset $X_W \subseteq Z$, which as verified later is distributed exactly as $X_{\text{III}} \cap W$. In order to determine whether or not a particular primary point $z \in Z_U$ with associated time t should be included in X_W, we need to consider the other marked points $(z_i, t_i) \in Y$ with $z_i \in B_R(z)$. Therefore, if $B_R(z)$ does not lie entirely in U, we first extend the primary Poisson point process Y_U to all of $B_R(z) \times [0, 1]$. If z is older than each such z_i (*i.e.*, $t_i > t$), then z is included in X_W. Even if it is not the oldest, it will still be retained if each older point $z_i \in B_R(z)$ (*i.e.*, $t_i < t$) is removed by some other retained point. To find out if that happens, we must examine recursively whether or not each such

Algorithm 1 `Perfect simulation of Matérn III`

Input: $W \subset \mathbb{R}^d$ of finite volume, $\lambda > 0$, $R > 0$
Output: $X_W = X_{\text{III}} \cap W$, a Matérn III process within the window W

$X_W \leftarrow \emptyset$, $U \leftarrow W$
draw $Y_U \leftarrow \mathsf{Poi}(U \times [0,1],\, \lambda)$
while $Y_U \cap \big(W \times [0,1]\big) \neq \emptyset$ **do**
  let (z,t) be the marked point in Y with smallest time
  draw $Y' \leftarrow \mathsf{Poi}\big([B_R(z) \setminus U] \times [0,1],\, \lambda\big)$
  $U \leftarrow U \cup B_R(z)$
  $Y_U \leftarrow Y_U \cup Y'$
  if $\big(\forall (z',t') \in Y'\big)\ \big(t < t'\big)$ **then**
    $Y_U \leftarrow Y_U \setminus \big(B_R(z) \times [0,1]\big)$
    if $z \in W$ **then** $X_W \leftarrow X_W \cup \{z\}$ **end if**
  end if
end while

z_i is retained in X_W.

For any marked point $(z,t) \in Y$, denote by $C(z,t)$ the 'directed Y-cluster' starting at (z,t), defined recursively as the union of (z,t) and the union of all directed Y-clusters $C(z_i,t_i)$ for $(z_i,t_i) \in \partial_<\big((z,t), Y\big)$, *i.e.*, with $\|z - z_i\| \leq R$ and $t_i < t$. These are the only marked points that might possibly influence whether or not z is retained in X_W. By Theorem 1 below, with probability one, each such directed cluster is finite for any $\lambda < \infty$. Consequently, Algorithm 1 will complete in finite time for any set $W \subset \mathbb{R}^d$ of finite volume.

3.2 Results

Before stating Theorem 1 we need to introduce some notation and results. For $(z,t) \in \mathbb{R}^d \times [0,1]$, let $Y^{(z,t)} = Y \cup \{(z,t)\}$. By stationarity (*i.e.*, the distribution of Y is invariant under translations in $\mathbb{R}^d$), for any fixed $(z,t) \in \mathbb{R}^d \times [0,1]$, we have the following: $(z,t) \notin Y$ almost surely; the expected size of the directed $Y^{(z,t)}$-cluster starting at $(z,t) \notin Y$ does not depend on z, so we can set

$$g(t) = \mathrm{E}[\#C(z,t)]; \tag{2}$$

and for an arbitrary Borel set $A \subseteq \mathbb{R}^d$, by Slivnyak-Mecke's theorem (Slivnyak, 1962; Mecke, 1967) (see also Møller and Waagepetersen, 2004, pp. 20–22),

$$\mathrm{E} \sum_{(z,t)\in Y\colon z\in A} \#C(z,t) = \lambda|A| \int_0^1 g(t)\ \mathrm{d}t, \tag{3}$$

where $|A|$ is the Lebesgue measure of A. Finally,

$$b = \lambda\omega_d R^d$$

denotes the expected number of points of $Z \cap B_R(z)$ for an arbitray fixed location $z \in \mathbb{R}^d$, where $\omega_d = \pi^{d/2}/\Gamma(1+d/2)$ is the volume of a unit ball.

Theorem 1. *We have the bound*

$$g(t) \le e^{b\,t}, \tag{4}$$

and with probability one, for all $(z,t) \in Y$, $\#C(z,t) < \infty$.

Before tackling the tight bound (4), it will be useful to have a weaker bound in place:

Lemma 1. *For some fixed* $B < \infty$ *and all* $0 \le t \le 1$, $g(t) \le B$.

Proof. First note that $g(0) = 1$ and that $g(t)$ is non-decreasing. Let Z^0 denote the projection of $Y^{(0,t)}$ onto $\mathbb{R}^d$, and $G(\lambda) \le \infty$ the expected size of the (undirected) Z^0-cluster containing 0. Since there is an upper bound on the number of $Z^0\setminus\{0\}$-clusters which has a member which is a neighbour to 0, it follows from Meester and Roy (1996, Theorem 3.2) that there exists $\lambda_c > 0$ such that $G(\lambda) < \infty$ for $\lambda \in (0, \lambda_c)$. Since the projection onto $\mathbb{R}^d$ of $Y^{(0,t)}$ is an undirected Z^0-cluster of the projection onto $\mathbb{R}^d$ of $Y^{(0,t)} \cap \big(\mathbb{R}^d \times [0,t]\big)$, the union of $\{(0,t)\}$ and a Poisson point process of intensity λt, we have $g(t) \le G(t\lambda)$. It follows that

$$g(t) \le G(\lambda_c/2) < \infty \quad \text{whenever } 0 \le t \le \lambda_c/(2\lambda). \tag{5}$$

Let $\{(z_1,t_1),\dots,(z_N,t_N)\}$ denote the older neighbours $\partial_<\big((0,t), Y^{(z,t)}\big)$ of $(0,t)$. Then $C(0,t)$ is the union of $\{(0,t)\}$ and $\cup_i C(z_i,t_i)$, so $\#C(0,t) \le 1 + \sum_{i=1}^N \#C(z_i,t_i)$, and taking expectations yields

$$g(t) \le 1 + \mathrm{E}\left[\sum_{i=1}^N \#C(z_i,t_i)\right].$$

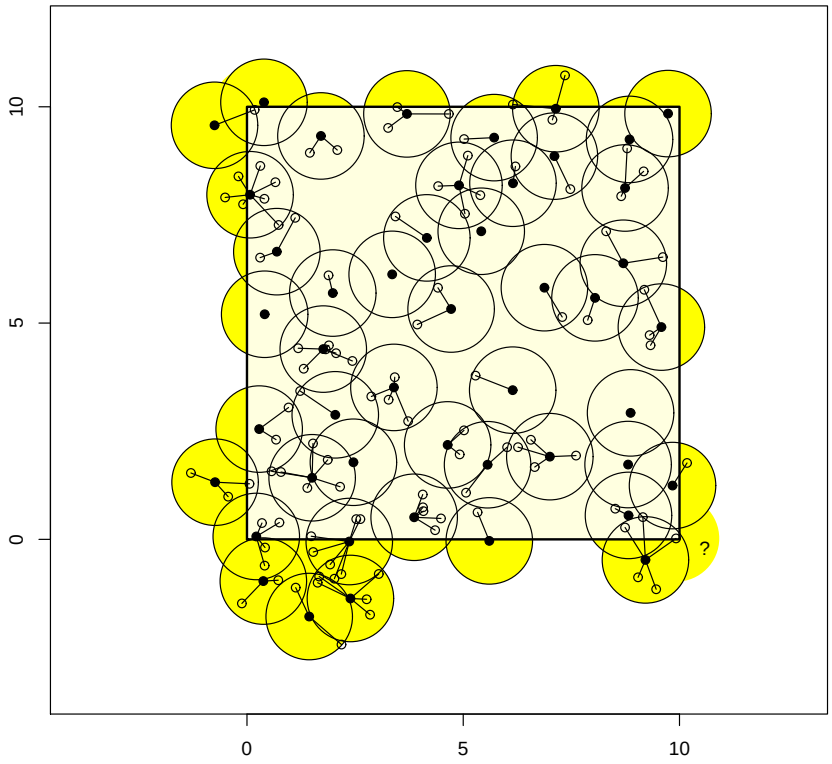

Figure 5: Illustration of Algorithm 1 when $W = [0, 10]^2$, $\lambda = 10$, and $R = 1$. Small filled circles are Matérn III points, which are the centers of the large circles of radii R. Small open circles are primary points, which are removed by Matérn III points, as indicated by the line segments. The question mark is a point outside W whose status was still uncertain when the algorithm terminated.

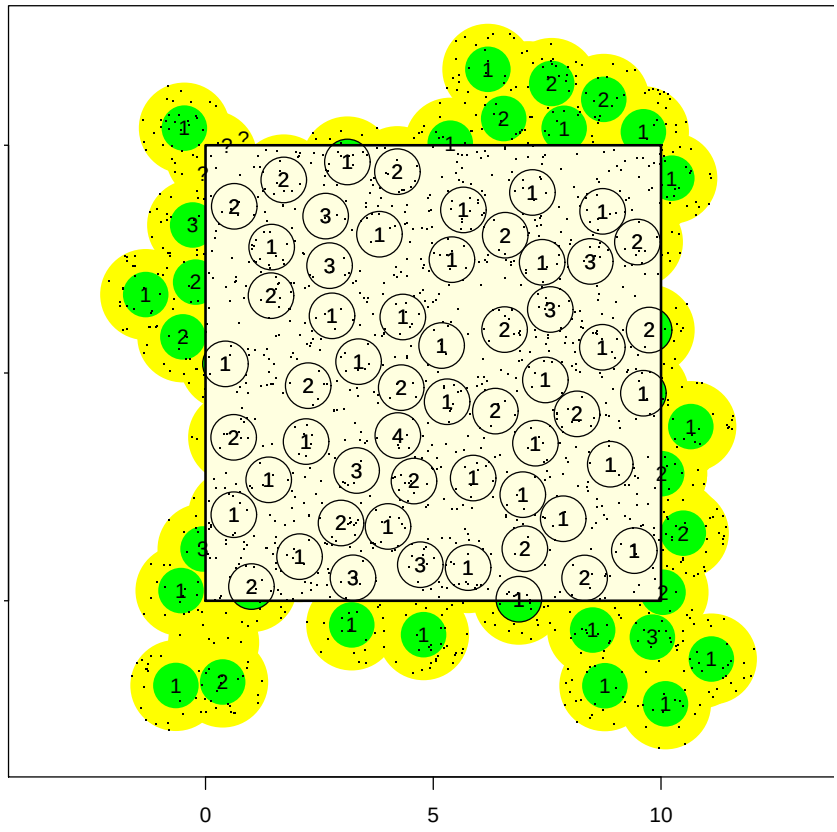

Figure 6: Illustration of Algorithm 1 when $W = [0, 10]^2$, $\lambda = 10$, and $R = 1$. Circled integers $i = 1, 2, \ldots$ are Matérn III points of the i^{th} generation $X^{(i)}$; circles have diameter R. The dots are the primary points that were removed by older Matérn III points within distance R. The shaded region outside W indicates the larger region U where additional primary points had to be generated to discover whether or not points within W would be retained. The question marks are points outside W whose status was still uncertain when the algorithm terminated.

Since $\{(z_1,t_1),\ldots,(z_N,t_N)\}$ is a Poisson process on $B_R(0)\times[0,t)$ with intensity λ, Slivnyak-Mecke's theorem and (2) imply that

$$\mathrm{E}\left[\sum_{i=1}^{N}\#C(z_i,t_i)\right]=\lambda\int_0^t\left[\int_{B_R(0)}\mathrm{E}[\#C(z,s)]\,\mathrm{d}z\right]\,\mathrm{d}s=b\int_0^t g(s)\,\mathrm{d}s.$$

Hence

$$g(t)\le 1+b\int_0^t g(s)\,\mathrm{d}s, \tag{6}$$

and so, for any $0<r<1$, since g is non-decreasing,

$$g(t)\le 1+b\,t\,\big[r\,g(rt)+(1-r)\,g(t)\big].$$

This implies that for $b(1-r)\le 1/2$, $0\le t\le 1$, and $k\in\mathbb{N}$,

$$\begin{aligned} g(t) &\le \frac{1}{1-bt(1-r)}+\frac{btr}{1-bt(1-r)}g(rt)\\ &\le 2+(2br)g(rt)\\ &\le 2\big[1+(2br)+\cdots+(2br)^{k-1}\big]+(2br)^k g(r^k t) \end{aligned} \tag{7}$$

where we have used induction to obtain (7). For $k\ge\log(2\lambda/\lambda_c)/\log(1/r)$, we have $r^k t\le\lambda_c/(2\lambda)$, and so by combining (5) and (7),

$$g(t)\le B:=2[1+(2br)+\cdots+(2br)^{k-1}]+(2br)^k G(\lambda_c/2)<\infty.$$

□

Now we turn to the theorem.

Proof of Theorem 1. Lemma 1 ensures that $g(s)$ is integrable over $[0,1]$, and so (6) and the integral form of Grönwall's inequality (Grönwall, 1919; Bellman, 1943) gives (4). The other assertion in Theorem 1 follows immediately by combining (3) and (4). □

Corollary 1. *With probability one, for any $i=1,2,\ldots$ and within any $Y^{(i)}$-cluster there will be at least one locally oldest member, and the cluster contains no infinite sequence of marked points $(z_1,t_1),(z_2,t_2),\ldots$ such that z_j is a younger neighbour to z_{j+1} for all $j=1,2,\ldots$.*

Proof. Follows immediately from Theorem 1. □

3.3 Extensions

This section considers an extension of the basic Matérn III process to the case where the ball $B_R(z_i)$ associated to each time t_i is replaced by $z_i + G_i = \{z_i + g : g \in G_i\}$, the translate by z_i of a random set $G_i \subseteq \mathbb{R}^d$. At the end of this section, we consider the inhomogeneous case where the intensity function of the underlying primary Poisson process is not constant.

Specifically, let Ω denote the space of random closed subsets of $\mathbb{R}^d$ equipped with the usual σ-algebra (see *e.g.* Stoyan et al., 1995, p. 94), and let Q denote a probability distribution for a random closed set. Let $G_1, G_2, \ldots$ be a sequence of i.i.d. random closed sets with distribution Q. This sequence is assumed to be independent of the Poisson process $Y = \{(z_1, t_1), (z_2, t_2), \ldots\}$ on $\mathbb{R}^d \times [0, 1]$ with intensity $\lambda > 0$. In other words, $Y^+ := \{(z_1, t_1, G_1), (z_2, t_2, G_2), \ldots\}$ is a Poisson process on $\mathbb{R}^d \times [0, 1] \times \Omega$ with intensity measure $\lambda \, \mathrm{d}z \, \mathrm{d}t \, \mathrm{d}Q(G)$. In the stochastic geometry literature, z_i is called a germ, $z_i + G_i$ a grain, and the union of the grains a germ-grain model or a Boolean model, where it is often assumed that G_i is compact (see *e.g.* Stoyan et al., 1995, p. 59 and p. 216). It turns out that the only condition we need in the sequel is that

$$b := \mathrm{E}[\#(Z \cap G_0)] = \lambda \mathrm{E}\left[|G_0|\right] \tag{8}$$

is finite, where G_0 follows Q and is independent of Y^+ (this implies the last equality in (8)). If, as previously in this paper, $G_0 = B_R(0)$ and $R > 0$ is fixed, then clearly $b = \lambda \omega_d R^d$ is finite. If instead R is a random variable, then condition (8) means that $\mathrm{E}[R^d] < \infty$. If $d = 2$ and G_0 is an ellipse with a random orientation and independent minor and major axes a and b, then (8) means that $\mathrm{E}[a]\mathrm{E}[b] < \infty$.

For any $(z_i, t_i, G_i) \in Y^+$, we think of $z_i + G_i$ as a 'demand space' and define

$$\partial_<\big((z_i, t_i, G_i), Y\big) = \{(z_j, t_j) \in Y : z_j \in z_i + G_i \text{ and } t_j < t_i\}$$

to be the subprocess of older neighbours to (z_i, t_i, G_i). By definition, the grain G_j of an older neighbour to (z_i, t_i, G_i) plays no role, explaining why we are only considering $\partial_<\big((z_i, t_i, G_i), Y\big)$ as a subprocess of the original primary Poisson process Y. This is advantageous when establishing Theorem 2 below, while the situation will be more complicated if we allowed older neighbours to depend on their grains.

Now, we construct the extended Matérn III process by retaining a point z_i only if it is not adjacent to an older neighbour that has already been

retained, cf. Section 2. In other words, a Matérn III point z_i arriving at time t_i 'demands' that $z_i + G_i$ is not containing any previously generated Matérn III point.

In a similar way as in Section 2, for any fixed $(z, t, G) \in \mathbb{R}^d \times [0, 1] \times \Omega$, define the directed $Y^{(z,t,G)}$-cluster starting with (z, t, G) and denote it $C(z, t, G)$. Note that $(z, t, G) \notin Y^+$ almost surely. Let

$$g(t) = \mathrm{E}[\#C(z, t, G_0)] \tag{9}$$

be the size of a directed cluster when G is replaced by the generic grain G_0, noticing that $g(t)$ does not depend on z. The following theorem bounds $g(t)$ above and establishes that the directed clusters $C(z_i, t_i, G_i)$, $i = 1, 2, \ldots$, are almost surely finite, meaning that our perfect simulation algorithm (Algorithm 1 modified to the case of the extended Matérn III process) completes in finite time.

Theorem 2. *The conclusions in Theorem 1 remain true for the extended Matérn III process.*

This is verified below. As in Section 3.1, it is easier to begin with weaker results.

Lemma 2. *If $0 \leq t < 1/b$, then $g(t) \leq 1/(1 - tb)$.*

Proof. The idea is to compare the directed cluster $C(0, t, G_0)$ to a branching process. Let $A_0 = \{(0, t)\}$, and for $i = 1, 2, \ldots$, let A_i denote the set of points in Y that reach $(0, t, G_0)$ in a directed path of i older neighbours in $C(0, t, G_0)$. For each $(z_j, t_j) \in A_i$, there exists at least one $(z_k, t_k) \in A_{i-1}$ such that $z_j \in z_k + G_k$ and $t_j < t_k \leq t$. Recall also that $G_0, G_1, G_2, \ldots$ are i.i.d. and independent of Y. Moreover, conditional on (z_k, t_k, G_k) with $(z_k, t_k) \in G_{i-1}$, the points $z_j \in Z$ with $t_j < t_k$ and $z_j \in z_k + G_k$ form a Poisson process on $z_k + G_k$ with intensity $t_k\lambda \leq t\lambda$. Consequently,

$$\mathrm{E}[\#A_i | A_{i-1}] \leq \sum_{(z_k,t_k)\in A_{i-1}} t\lambda \mathrm{E}\left[|G_k|\right] = tb\#A_{i-1}.$$

Taking the conditional expectation over the points in A_{i-1} given $\#A_{i-1}$, we obtain

$$\mathrm{E}[\#A_i | \#A_{i-1}] \leq tb\#A_{i-1}.$$

Using that $\#A_0 = 1$ supplies the base case of an induction that yields $\mathrm{E}[\#A_i] \leq (tb)^i$. So, for $0 \leq t < 1/b$,

$$g(t) = \sum_{i=0}^{\infty} \mathrm{E}[\#A_i] \leq \sum_{i=0}^{\infty} (tb)^i = 1/(1-tb).$$

□

Lemma 3. *There exists a fixed $B < \infty$ such that for all $t \in [0,1]$, $g(t) \leq B$. Moreover, (6) remains true.*

Proof. As in the proof of Lemma 1,

$$g(t) \leq 1 + \mathrm{E}\left[\sum_{i=1}^{N} \#C(z_i, t_i, G_i)\right], \tag{10}$$

where $\{(z_1, t_1), \ldots, (z_N, t_N)\}$ are the older neighbours of $(0, t, G_0)$. Conditional on G_0, these older neighbours form a Poisson process on $G_0 \times [0,t) \times \Omega$. Hence

$$\begin{aligned}
\mathrm{E}\left[\sum_{i=1}^{N} \#C(z_i, t_i, G_i)\right] &= \mathrm{E}\left[\mathrm{E}\left[\sum_{i=1}^{N} \#C(z_i, t_i, G_i)\middle| G_0\right]\right] \\
&= \lambda \int_0^t \mathrm{E}\left[\int_{G_0}\int_{\Omega} \mathrm{E}\left[\#C(z,s,G)|G_0\right] \,\mathrm{d}Q(G)\,\mathrm{d}z\right] \,\mathrm{d}s \qquad (11) \\
&= \lambda \int_0^t \mathrm{E}\left[\int_{G_0}\int_{\Omega} \mathrm{E}\left[\#C(z,s,G)\right] \,\mathrm{d}Q(G)\,\mathrm{d}z\right] \,\mathrm{d}s \qquad (12) \\
&= \lambda \int_0^t g(s)\,\mathrm{E}\left[\int_{G_0} \mathrm{d}z\right] \,\mathrm{d}s \qquad (13) \\
&= b \int_0^t g(s)\,\mathrm{d}s, \qquad (14)
\end{aligned}$$

using Slivnyak-Mecke's theorem and Fubini's theorem in (11), the fact that G_0 is independent of Y^+ in (12), (9) in (13), and (8) in (14). Consequently, we have again established (6). The remainder of the proof can then be completed as in Lemma 1, using instead of (5) the fact that

$$g(t) \leq 1/[1 - 1/(2b)] \quad \text{whenever } 0 \leq t \leq 1/(2b). \tag{15}$$

Here (15) follows from Lemma 2. □

With Lemma 3 in hand, the proof of Theorem 2 is identical to that of Theorem 1.

Inhomogeneous intensity Now, consider the further extension where the intensity λ is replaced by a locally integrable intensity function $\lambda(z)$ so that Y^+ is a Poisson process on $\mathbb{R}^d \times [0,1] \times \Omega$ with intensity measure $\lambda(z)\,\mathrm{d}z\,\mathrm{d}t\,\mathrm{d}Q(G)$. In this case, $b(z) = \mathrm{E}[\#(Z \cap (z + G_0))]$ and $g(t,z) = \mathrm{E}[\#C(z,t,z+G_0)]$ are no longer independent of z, and so new definitions are needed:

$$b := \sup_z \mathrm{E}\left[\#(Z \cap (z + G_0))\right],$$
$$g(t) := \sup_z \mathrm{E}\left[\#(C(z,t,z+G_0)\right].$$

When λ is a constant function these new definitions reduce to the previous ones. Assume that $b < \infty$, noticing that

$$b = \sup_z \mathrm{E}\left[\int_{G_0} \lambda(x-z)\,\mathrm{d}x\right].$$

In the proofs of Lemmas 2 and 3 some equalities change to less than or equal to statements, but otherwise the proofs remain unchanged. Hence Theorem 2 still holds using these more general definitions of b and $g(t)$.

3.4 Speeding up the algorithm

In Algorithm 1, when the point z with time stamp t is considered, all points in the primary Poisson process within distance R to z are generated. This, however, is wasteful, since only those neighbours that have a time stamp smaller than t can possibly affect z. This ball of radius R about z, $B_R(z)$, is then added to the set U.

By only generating points in $B_R(z)$ with times stamps smaller than t, the algorithm becomes much faster and gives rise to our Algorithm 2. The set U in Algorithm 1 is replaced in Algorithm 2 by a subset V of space-time, and when the points with time stamp less than t are generated, the space-time cylinder $B_R(z) \times [0,t]$ is added to V. Generation of points in $(B_R(z) \times [0,t]) \setminus V$ is accomplished by first generating points in $B_r(z) \times [0,t]$, and then retaining those points that lie outside of V. Using the same primary Poisson process in the two algorithms, Algorithm 2 generates fewer points

than Algorithm 1. In fact, for high primary intensities λ the distribution of times $\{t_i\}$ of retained points is clustered close to zero so the reduction in running time is substantial. When $b > 1000$ this reduction often exceeded three orders of magnitude in our trials.

Algorithm 2 `Perfect simulation of Matérn III`

Input: $W \subset \mathbb{R}^d$ of finite volume, $\lambda > 0$, $R > 0$
Output: $X_W = X_{\text{III}} \cap W$, a Matérn III process within the window W

$X_W \leftarrow \emptyset$, $V \leftarrow W \times [0,1]$
draw $Y_V \leftarrow \mathsf{Poi}(V, \lambda)$
while $Y_V \cap (W \times [0,1]) \neq \emptyset$ **do**
  let (z,t) be the point in Y_V with smallest time
  draw $Y' \leftarrow \mathsf{Poi}\big([(B_R(z) \times [0,t]) \setminus V], \lambda\big)$
  $V \leftarrow V \cup (B_R(z) \times [0,t])$
  $Y_V \leftarrow Y_V \cup Y'$
  if $Y' = \emptyset$ **then**
    $Y_V \leftarrow Y_V \setminus \big(B_R(z) \times [0,1]\big)$
    if $z \in W$ **then** $X_W \leftarrow X_W \cup \{z\}$ **end if**
  end if
end while

4 Packing densities

For a stationary hard core process X in $\mathbb{R}^d$ with hard core $R > 0$ and intensity $\rho < \infty$, the *packing density* τ is the volume fraction taken up by the (disjoint) balls of radius $R/2$ centered at the points; for an arbitrary Borel set $A \subset \mathbb{R}^d$ of positive and finite Lebesgue measure $|A|$,

$$\tau = \frac{1}{|A|} \mathrm{E} \left| \bigcup_{x \in X} \big(B_{R/2}(x) \cap A\big) \right|,$$

which by stationarity does not depend on the choice of A. By Campbell's theorem (see, *e.g.*, Stoyan et al., 1995, *p.* 103),

$$\tau = \rho \omega_d (R/2)^d. \tag{16}$$

Furthermore, for Z a stationary Poisson process with intensity λ, the Boolean model $Z_R = \cup_{z\in Z} B_{R/2}(z)$ has expected volume fraction

$$\tau_0 := \mathrm{E}|Z_R \cap A|/|A| = 1 - \exp\left(-\lambda\omega_d (R/2)^d\right).$$

Using an obvious notation, we obtain for Matérn I–III generated by a primary Poisson process Y with intensity $\lambda > 0$ the following relation between the packing densities

$$\tau_{\mathrm{I}} < \tau_{\mathrm{II}} < \tau_{\mathrm{III}} < \tau_0,$$

cf. Proposition 1. Note that τ_i ($i =$ I, II, III) depends on (λ, R) only through $b = \lambda\omega_d R^d$. By stationarity in $\mathbb{R}^d$ and using (16), we have

$$\tau_i = \left(b/2^d\right) \int_0^1 p_i(t)\ \mathrm{d}t, \quad i = \mathrm{I},\ \mathrm{II},\ \mathrm{III}, \tag{17}$$

where $p_i(t)$ is the probability that $0 \in \mathbb{R}^d$ with associated time t is not i-thinned by the marked points in Y ($i =$ I,II,III).

4.1 Packing densities for Matérn I and II

Since b is the expected number of primary points in a ball of radius R, $p_{\mathrm{I}}(t) = \exp(-b)$ and $p_{\mathrm{II}}(t) = \exp(-bt)$, and hence by (17),

$$\tau_{\mathrm{I}} = b\, e^{-b}/2^d, \quad \tau_{\mathrm{II}} = (1 - e^{-b})/2^d.$$

Evidently τ_{I} takes its maximum when $b = 1$, and τ_{II} approaches its maximum as $b \to \infty$, with

$$\sup \tau_{\mathrm{I}} = 2^{-d}/e, \quad \sup \tau_{\mathrm{II}} = 2^{-d}.$$

4.2 Packing density for Matérn III

4.2.1 Analytical results

Suppose that $\{(z_1, t_1), \ldots, (z_N, t_N)\}$ is the Poisson process of primary marked points in $B_R(0)\times[0, t)$; note that N is Poisson distributed with mean bt. Conditional on these primary marked points, for $N = n \geq 1$, let $q_n(z_1, t_1, \ldots, z_n, t_n)$ denote the probability that every (z_i, t_i) $(i = 1, \ldots, n)$ is non-retained after III-thinning (we say shortly that (z_i, t_i) is III-thinned) by marked points in $Y \setminus (B_R(0) \times [0, 1])$. If $(0, t)$ is not III-thinned by Y and $t_{(1)} < \ldots < t_{(n)}$

are the ordered times, then by induction on $i = 1, \ldots, n$ we see that each $(z_{(i)}, t_{(i)})$ must be III-thinned by some Matérn III points outside $B_R(0)$ with marks less than t. Thus $p_{\text{III}}(t)$ in Equation (17) is given by

$$p_{\text{III}}(t) = e^{-bt}\left[1 + \sum_{n=1}^{\infty} \frac{(bt)^n}{n!} \int \cdots \int q_n(z_1, t_1, \ldots, z_n, t_n) \right. \tag{18}$$
$$\left. \mathrm{d}\nu_t(z_1, t_1) \cdots \mathrm{d}\nu_t(z_n, t_n)\right],$$

where ν_t denotes the uniform distribution on $B_R(0) \times [0, t]$. The earlier lower bound $\tau_{\text{III}} > \tau_{\text{II}}$ follows simply by ignoring the sum in (18). It seems challenging to express $q_n(z_1, t_1, \ldots, z_n, t_n)$ in closed form, and extremely difficult even to derive a lower bound on $q_1(z_1, t_1)$, since (z_1, t_1) has to be III-thinned by some $(z_2, t_2) \in Y \cap ([B_R(z_1) \setminus B_R(0)] \times [0, t_1))$ which in turn is not III-thinned. We have also not been successful in establishing a useful upper bound on $q_n(z_1, t_1, \ldots, z_n, t_n)$.

4.2.2 Simulated results

Algorithm 2 was implemented in the `R` programming environment (R Development Core Team, 2006) and was run on a 2.66GHz dual quad-core Xeon-based desktop computer at a range of primary intensities, evenly spaced on a logarithmic scale. All simulations used radius $R = 1$ on a 10×10 square window W. Running times varied from microseconds per run at the lowest value of $b = 1.0$ to five hours per step for the highest value of $b = 10^{5.5}$. Memory limitations prevented the exploration of higher values of b.

The solid line in Figure 7 gives the estimated packing density τ_{III} of the Matérn III process as a function of b. Circles indicate values of b at which simulations were run. Short vertical lines give 99% uncertainty range reflecting simulation variability, which was negligible except for the highest densities. Dashed lines indicate the approximate packing density of points in generations 1–7; no points of higher generations were observed. Generation 1 has the Matérn II distribution, and quickly reaches its asymptotic value of $\tau_{\text{II}} = 1/4$ in $d = 2$ dimensions.

Feder (1980) offered empirical evidence for his conjecture that the error in estimating the packing density for the RSA process with n attempts to place a new disk decreased like $n^{-1/2}$ in two dimensions. Figure 8 presents a plot of our estimated packing density against the inverse square root of b for the

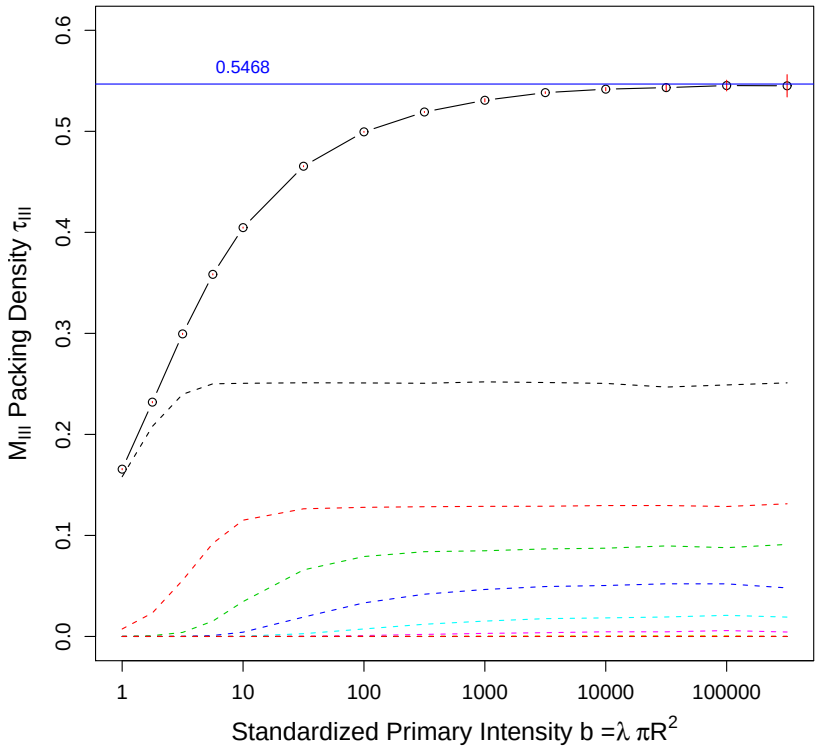

Figure 7: Illustration of dependence of Matérn III packing density τ_{III} on standardized intensity of primary process (solid curve). Dashed curves are contributions of points in $X^{(i)}$ for $i = 1, 2, ..., 7$ (top to bottom). Short vertical lines at nodes are 99% intervals.

Matérn III process. A linear regression fit to the values from the highest four intensities is presented as a dashed line; its intercept, the 'Feder extrapolation' of the packing density to infinite intensity $1/\sqrt{b} \approx 0$, is 0.5468 ± 0.00044, consistent with reported estimates of RSA intensity at the jamming limit (0.547 ± 0.002 by Feder (1980, *p.* 240), 0.5471 ± 0.0051 by Hinrichsen, Feder, and Jøssang (1986, *p.* 801), 0.5467 ± 0.0003 by Meakin and Jullien (1992, *p.* 2030), 0.5473 ± 0.0009 by Tanemura (1979, *p.* 362), 0.5444 ± 0.0024 by Tory, Jodrey, and Pickard (1983, *p.* 444)).

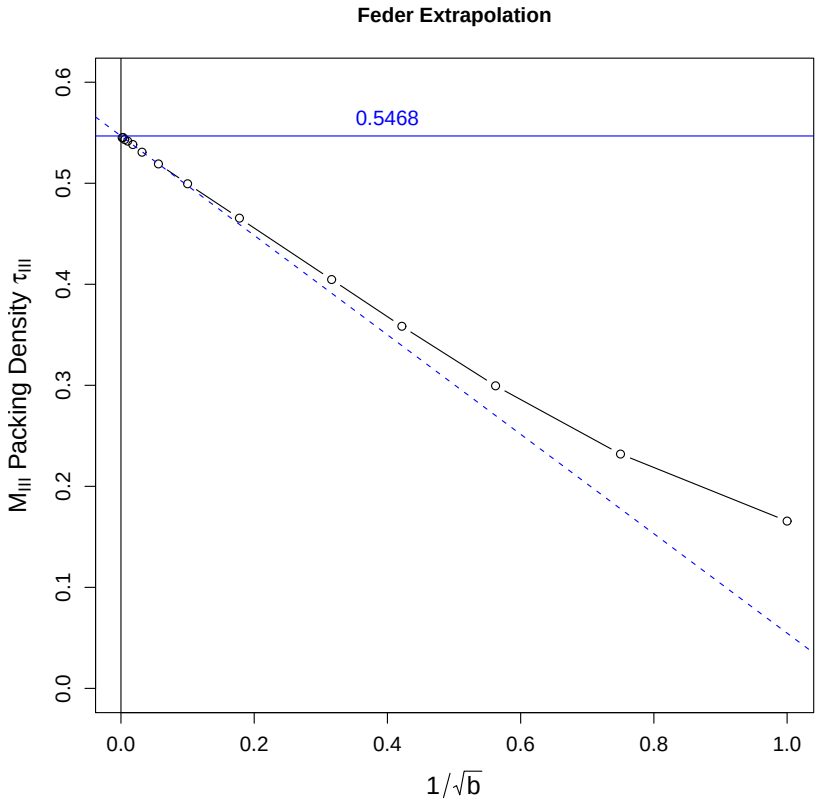

Figure 8: Extrapolation estimate of τ_{III} following Feder (1980).

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References

Bellman, R., 1943. The stability of solutions of linear differential equations. Duke Math. J. 10 (4), 643–647.

Döge, G., 2001. Perfect simulation for random sequential adsorption of d-dimensional spheres with random radii. Journal of Statistical Computation and Simulation 69 (2), 141–156.

Feder, J., 1980. Random sequential adsorption. Journal of Theoretical Biology 87 (3), 273–254.

Finegold, L., Donnell, J. T., Mar. 1979. Maximum density of random placing of membrane particles. Nature 278 (5703), 443–445.

Grönwall, T. H., 1919. Note on the derivative with respect to a parameter of the solutions of a system of differential equations. Ann. Math. 20 (2), 292–296.

Hinrichsen, E. L., Feder, J., Jøssang, T., 1986. Geometry of random sequential adsorption. Journal of Statistical Physics 44 (5–6), 793–827.

Huber, M. L., Wolpert, R. L., 2009. Likelihood-based inference for Matérn type III repulsive point processes. Adv. Appl. Probab.Forthcoming.

Matérn, B., 1960. Spatial variation. stochastic models and their application to some problems in forest surveys and other sampling investigations. Medd. Statens Skogsforskningsinstitut 49 (5), 1–144.

Matérn, B., 1986. Spatial Variation, 2nd Edition. Vol. 36 of Lecture Notes in Statistics. Springer-Verlag, New York, NY, (first edition published 1960 by Statens Skogsforsningsinstitut, Stockholm).

Meakin, P., Jullien, R., Aug. 1992. Random-sequential adsorption of disks of different sizes. Physical Review A 46 (4), 2029–2038.

Mecke, J., 1967. Stationire zufallige Masse auf localcompakten Abelischen Gruppen. Z. Wahrscheinlichkeit. 9 (1), 36–58.

Meester, R., Roy, R., 1996. Continuum Percolation. Vol. 119 of Cambridge Tracts in Mathematics. Cambridge Univ. Press, Cambridge, UK.

Møller, J., Waagepetersen, R. P., 2004. Statistical Inference and Simulation for Spatial Point Processes. Chapman & Hall/CRC, Boca Raton, FL.

Pálasti, I., 1960. On some random space filling problems. Publ. Math. Inst. Hungar. Acad. Sci. 5, 353–359.

Penrose, M. D., 2001. Random parking, sequential adsorption, and the jamming limit. Communications in Mathematical Physics 218 (1), 153–176.

Propp, J. G., Wilson, D. B., 1996. Exact sampling with coupled markov chains and applications to statistical mechanics. Random Struct. Algor. 9 (1-2), 223–252.

R Development Core Team, 2006. R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, AT. URL `http://www.R-project.org`

Ripley, B. D., 1981. Spatial Statistics. Wiley Series in Probability and Statistics. John Wiley & Sons, New York, NY.

Schaaf, P., Voegel, J.-C., Senger, B., 1998. Irreversible deposition/adsorption processes on solid surfaces. Annales de Physique 23 (6), 1–89.

Schreiber, T., Penrose, M. D., Yukich, J. E., 2007. Gaussian limits for multidimensional random sequential packing at saturation. Communications in Mathematical Physics 272, 167–183.

Slivnyak, I. M., 1962. Some properties of stationary flows of homogeneous random events. Teor. Veroyat. Primen. 7, 347–352, (in Russian). English translation: Theory Prob. Appl. 7, 336-341.

Solomon, H., 1967. Random packing density. In: Le Cam, L. M., Neyman, J. (Eds.), Proceedings of the Fifth Berkeley Symposium on Mathematical Statistics and Probability. Vol. 3: Physical Sciences. University of California Press, Berkeley, CA, pp. 119–134.

Stoyan, D., Kendall, W. S., Mecke, J., 1995. Stochastic Geometry and Its Applications, 2nd Edition. John Wiley & Sons, Chichester, West Sussex, UK.

Stoyan, D., Schlather, M., 2000. Random sequential adsorption: relationship to dead leaves and characterization of variability. J. Stat. Phys. 100 (5/6), 969–979.

Tanemura, M., 1979. On random complete packing by discs. Annals of the Institute of Statistical Mathematics B 31 (2), 351–365.

Tory, E. M., Jodrey, W. S., Pickard, D. K., 1983. Simulation of random sequential adsorption: Efficient methods and resolution of conflicting results. Journal of Theoretical Biology 102 (3), 439–445.