

## A NON-MONOTONE CFTP PERFECT SIMULATION METHOD

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*Abstract:* In this paper, we present a non-monotone *coupling from the past* (CFTP) method for obtaining perfect samples from the equilibrium distribution of a Markov chain. This method requires no monotone structure that is difficult to define in practice. We also apply the non-monotone CFTP method to general non-monotone birth-death processes and area-interaction point processes.

*Key words and phrases:* Area-interaction point processes, birth-death processes, CFTP, MCMC, monotone, non-monotone, perfect simulation.

### 1. Introduction

The Markov chain Monte Carlo (MCMC) method has been used extensively in obtaining a sample from a complicated multivariate probability distribution  $\pi$ . This method can be implemented as follows: (a) define an ergodic Markov chain  $X$  with stationary distribution  $\pi$ ; (b) start the chain in some arbitrary state and run the chain for a long time, say  $M$  steps, where  $M$  is a large integer; (c) output the final state  $x_M$ . The ergodicity of the Markov chain guarantees that, if  $M$  is sufficiently large, then the distribution of  $X_M$  is close to  $\pi$ .

One of the problems with the MCMC approach is that it may be difficult to determine how large  $M$  should be. It is now well-known that *perfect simulation* methods, first proposed by Propp and Wilson (1996), can be used to solve this problem. A perfect simulation algorithm is one which can self-verify whether the simulated chain has reached stationarity and thus produce exact samples from the equilibrium distribution  $\pi$ .

The development in the area of perfect simulation has been rapid. There are two main types of methods: one is based on the CFTP idea proposed by Propp and Wilson (1996), the other the *interruptible method* proposed by Fill (1998). In the following we concentrate on CFTP methods. Most of the CFTP methods depend on a partial order defined in a state space, so they are called monotone CFTP methods. Dominated CFTP is a variant of CFTP developed by Kendall (1998) that permits perfect simulation of a general class of point processes (also see Kendall and Møllér (2000)). Dominated CFTP has an importance going

beyond point processes since it allows applications of CFTP to a wide class of non-uniformly ergodic Markov chains which need not be monotonic. Kendall and Thönnies (1999) used dominated CFTP to carry out perfect simulations in stochastic geometry, showing how to get perfect samples from Boolean models conditioned to cover a finite set of points. Extended state-space CFTP presented by Cai and Kendall (2002) can be used to obtain a perfect sample from the equilibrium distribution  $\pi$  of a discrete or continuous time Markov chain which is not uniformly ergodic and which takes values in a state space, without assuming any monotonicity. However, we need to explore the monotonicity in an extended state space. Cai (2002) also studied how the rates of convergence for Gibbs fields depend on the interaction and the kind of scanning used by monotone CFTP methods. Wilson (2000) presented a read-once perfect simulation method and applied it to locally stable point processes. His method is related to CFTP, but only runs the Markov chain forward in time and never restarts it at previous times in the past. However, the method still depends heavily on a monotone structure.

Another variant of CFTP was developed in the direction of not assuming any monotonicity at all. For example, Murdoch and Green (1998) extended CFTP to various MCMC samplers on a continuous state space. Their methods do not depend on any monotonicity structures but are not applicable to point processes. Fernández, Ferrari and Garcia (2002) presented a perfect simulation algorithm for measures that are absolutely continuous with respect to some Poisson processes and that can be obtained as invariant measures of birth-death processes. Their algorithm does not require monotonicity and can directly provides samples of an infinite-volume measure, but it seems difficult to apply them to other problems. Huber (1998) and Harvey and Neal (2000) have shown that the CFTP method may be generalized by using a single summary state rather than a pair of extremal states. This single state summarizes one's knowledge of the possible states of the system, allowing the state of some subsystems to be uncertain. Childs, Patterson and Mackay (2001) developed a summary state CFTP method for Ising models.

The purpose of this paper is to present a general non-monotone CFTP method and to show its applications through general birth-death processes and area-interaction point processes.

After reviewing the basic form of the monotone CFTP method presented by Propp and Wilson (1996) in Section 2, we give a general description of the non-monotone CFTP method in Section 3. The application of the new method to a birth-death process is given in Section 4, to area-interaction point processes in Section 5. Finally, conclusions and comments are given in Section 6.

## 2. The Simplest form of Monotone CFTP Method

The standard MCMC method is to run a Markov chain from time, say,  $t = 0$  to infinity. Since this is impossible, the algorithm has to stop when the chain has been run long enough. It is difficult to know then whether the output is a sample from the equilibrium distribution of the Markov chain or not. The CFTP method provides a way to determine when the algorithm should stop and guarantees that, under certain conditions, the output at time 0 is a sample from the equilibrium distribution of the Markov chain.

Specifically, the simplest CFTP method (Propp and Wilson (1996)) runs a Markov chain as follows. Suppose the state space of the Markov chain is finite. Start the simulation at time  $-T$  from all possible starting points and run these chains till time 0. If all the chains coalesce at the same state by time 0 then the simulation finishes. The output is a sample from the equilibrium distribution of the Markov chain. If all the paths started at time  $-T$  have not coalesced by time 0, choose a new value  $-T_1 < -T$  and restart the simulation from time  $-T_1$ . In this, re-use the random numbers  $u_t$  which are used in the previous stage of the simulation. The process should be continued until all chains coalesce by time 0.

To deal with the case when the state space is very large or infinite, a monotone CFTP method can be used (Propp and Wilson (1996)). Here suppose the state space  $S$  admits a natural partial order  $\leq$ , and that there exist  $\hat{0}$  and  $\hat{1}$  in  $S$  such that  $\hat{0} \leq x \leq \hat{1}$  for all  $x \in S$ . Furthermore suppose we can define an update rule  $\phi$  such that  $\phi(x, u) \leq \phi(y, u)$  for all  $u$  whenever  $x \leq y$ . Then we have the simplest form of monotone CFTP algorithm in Table 1.

Table 1. Simplest form of Monotone CFTP algorithm.

<p><b>Monotone CFTP</b>(<math>-T</math>):</p> <p><math>upper \leftarrow \hat{1}</math></p> <p><math>lower \leftarrow \hat{0}</math></p> <p>for <math>t = -T, \dots, 1</math></p> <p style="padding-left: 2em;"><math>upper \leftarrow \phi(upper, u_t)</math></p> <p style="padding-left: 2em;"><math>lower \leftarrow \phi(lower, u_t)</math></p> <p><b>if</b> <math>upper = lower</math></p> <p style="padding-left: 2em;"><b>output</b> <math>upper</math></p> <p><b>else</b></p> <p style="padding-left: 2em;"><b>Monotone CFTP</b>(<math>-2T</math>)</p>
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## 3. Non-monotone CFTP Method

To develop a monotone CFTP algorithm we need to explore a certain monotone structure in the original state space or in an extended state space of the

Markov chain. Unfortunately there are many cases in which the monotonicity does not exist or is difficult to define. Therefore it is important to develop a method which does not require monotone structures.

Let us look at the monotone CFTP method in another way. Let  $X = \{X_t\}$  be the Markov chain run from its equilibrium distribution  $\pi$ , corresponding to running from time  $-\infty$ . Let  $X^{\max} = \{X_t^{\max}\}$  and  $X^{\min} = \{X_t^{\min}\}$  be the upper and lower chains run from  $t = -T$ . Then for  $t_0 > -T$ , we have

$$X_{t_0}^{\min} \leq X_{t_0} \leq X_{t_0}^{\max}.$$

Let  $S_{t_0}$  be the set of all states that lie between  $X_{t_0}^{\min}$  and  $X_{t_0}^{\max}$ . Then  $S_{t_0} = W_{t_0} \cup V_{t_0}$ , where  $W_{t_0} = \{X_{t_0}\}$  and  $V_{t_0} = S_{t_0} \setminus \{X_{t_0}\}$ . So  $W_{t_0}$  contains an exact sample of  $\pi$ , we call  $W_{t_0}$  the certain part of  $X$  at  $t_0$ ;  $V_{t_0}$  contains other states of the chain, we call it the uncertain part of  $X$  at  $t_0$ .

Although, theoretically, we know  $X_{t_0}$  is an exact sample of  $\pi$ , it is not easy to pick up  $X_{t_0}$  from the set  $S_{t_0}$  if it contains more than one state. However, if the two extreme chains have coalesced by time 0, then  $X_0^{\min} = X_0 = X_0^{\max}$ , so,  $V_0 = \emptyset$  and we obtain a perfect sample.

Monotone CFTP provides a way to determine when the uncertain part of  $X$  has disappeared. Although this way to look at CFTP has been explored before, little has been done on how to use it to construct non-monotone CFTP algorithms. In the following we give general principles of the non-monotone CFTP method, then give some applications.

To construct a non-monotone CFTP we run a single chain, rather than two extreme chains. Let  $X_t^{-T}$  be the state of a Markov chain  $X$  at time  $t$  starting from time  $-T$ . If the chain has reached its equilibrium by time  $t_0$ , then  $X_{t_0}^{-T}$  must contain all the properties of being an exact sample from the equilibrium. We view the single state  $X_{t_0}^{-T}$  as a union of certain and uncertain parts, once the uncertain part disappears by time 0 we have a perfect sample.

Specifically, a general non-monotone CFTP can be constructed as follows.

- Start the chain from time  $-T$  and run it to time 0.
- For  $-T \leq t \leq 0$ , let  $X_t^{-T} = W_t^{-T} \sqcup V_t^{-T}$ , where  $\sqcup$  is the union over the two types of information.
- If by time 0 the uncertain part  $V_0^{-T}$  of  $X_0^{-T}$  disappears, we have a perfect sample  $X_0^{-T} = W_0^{-T}$  from the equilibrium distribution of  $X$ .
- Otherwise, we go back further in time and re-run the chain until the uncertain part  $V_t^{-T}$  of  $X_t^{-T}$  disappears by time 0.

The detailed construction of the non-monotone CFTP algorithm is problem specific. In the following we apply the general method to two examples: a general birth-death process and an area-interaction point process. In the two examples we show both the monotone and the non-monotone constructions, and we see how to express the two types of information in different problems.

#### 4. General Birth-death Processes

Suppose  $X$  is a continuous-time Markov chain on the non-negative integers such that each individual departs at a constant rate  $\mu$ , and individuals arrive at rate  $\alpha(X)$  depending on the current population. That is, the Markov chain has transition rates

$$\begin{aligned} X &\rightarrow X + 1 \text{ at rate } \alpha(X), \\ X &\rightarrow X - 1 \text{ at rate } \mu X. \end{aligned} \tag{1}$$

If for all  $X$  we have  $\alpha(X) > 0$ ,  $\sum_{j=0}^{\infty} v_j < \infty$  with  $v_0 = 1$ , and  $v_j = (\alpha(0) \cdots \alpha(j-1)) / (\mu^j j!)$  for  $j \geq 1$ , then the stationary distribution of  $X$  is given by

$$\pi_j = \frac{v_j}{\sum_{i=0}^{\infty} v_i}, \quad j = 0, 1, 2, \dots$$

We want to sample from  $\pi = (\pi_0, \pi_1, \dots)$ .

##### 4.1. Monotone CFTP approach to the birth-death processes

Kendall (1996) showed how to construct a dominated CFTP algorithm for the birth-death process under the monotone condition

$$0 < \alpha(0) \leq \alpha(X) \leq \alpha(X + 1) \leq \lambda. \tag{2}$$

Thus, given  $\lambda$ , we define another process  $Y$  such that  $Y \rightarrow Y + 1$  at rate  $\lambda$  and  $Y \rightarrow Y - 1$  at rate  $\mu Y$ . It is easy to prove that the  $Y$  process satisfies detailed balance and has an equilibrium distribution which is Poisson of mean  $\lambda/\mu$ .

Now let  $\mathcal{L}$  be the ordered set of birth-death times of  $Y$  on  $[-T, 0]$  when  $Y$  is simulated from its equilibrium distribution. For each time incidence  $t$  in  $\mathcal{L}$  we attach a mark  $p_t$  to it, where  $p_t$  is a value randomly chosen in the interval  $(0, 1)$ . Let  $X_t^{-T, \max}$  ( $X_t^{-T, \min}$ ) be the value of the maximum (minimum) process at time  $t$  starting from time  $-T$ . Then under (2) we can define the evolution of the maximum and minimum processes of  $X$  as follows.

- At time  $-T$  set  $X_{-T}^{-T, \max} = Y_{-T}$  and  $X_{-T}^{-T, \min} = 0$ .
- For  $t \in \mathcal{L}$ ,

if  $t$  is a birth time of  $Y$ ,

$$\begin{aligned} X_t^{-T,\max} &= X_{t-}^{-T,\max} + 1 & \text{if } p_t &\leq \frac{\alpha(X_{t-}^{-T,\max})}{\lambda}, \\ X_t^{-T,\min} &= X_{t-}^{-T,\min} + 1 & \text{if } p_t &\leq \frac{\alpha(X_{t-}^{-T,\min})}{\lambda}; \end{aligned}$$

if  $t$  is a death time of  $Y$ ,

$$\begin{aligned} X_t^{-T,\max} &= X_{t-}^{-T,\max} - 1 & \text{if } p_t &\leq \frac{X_{t-}^{-T,\min}}{Y_{t-}}, \\ X_t^{-T,\min} &= X_{t-}^{-T,\min} - 1 & \text{if } p_t &\leq \frac{X_{t-}^{-T,\max}}{Y_{t-}}. \end{aligned}$$

- If  $X_0^{-T,\max} = X_0^{-T,\min}$  we output  $X_0^{-T,\max}$ . Otherwise we go back further in time and repeat the above procedure until coalescence occurs.

Note that in the above algorithm  $Y$  should be simulated from its equilibrium distribution and both maximum and minimum processes use the same marks  $p_t$ . Coalescence eventually occurs for large enough  $T$ . For example, when  $Y = 0$  coalescence occurs. Furthermore, it is not difficult to prove that after coalescence the chain will evolve with the transition rates given by (1) and we have a perfect sample from the equilibrium distribution of  $X$ .

The monotone condition (2) plays a crucial role in the above construction. It guarantees that if there is a birth in the minimum process, then there must be a birth in the maximum process, because the acceptance probabilities satisfy

$$\frac{\alpha(X_{t-}^{-T,\min})}{\lambda} \leq \frac{\alpha(X_{t-}^{-T,\max})}{\lambda}.$$

On the other hand, if there is a death in the maximum process, then there must be a death in the minimum process, because

$$\frac{X_{t-}^{-T,\min}}{Y_{t-}} \leq \frac{X_{t-}^{-T,\max}}{Y_{t-}}.$$

So at any time  $-T \leq t \leq 0$ , we always have  $X_t^{-T,\min} \leq X_t^{-T,\max}$ . The condition (2) also guarantees that the virtual chain (the chain starting from  $-\infty$ ) is sandwiched between the two extreme chains (The details can be found in Kendall (1996)).

#### 4.2. Non-monotone CFTP Approach to the Birth-death Processes

Suppose the overall birth rate  $\alpha(X)$  does not satisfy (2) but  $0 < \alpha(X) \leq \lambda$ . To construct a non-monotone CFTP method in this case we need to express the

two parts of  $X_t$  clearly. First we write  $X_t^{-T} = W_t^{-T} + V_t^{-T}$ , where  $X_t^{-T}$  is the number of all possible individuals in the population at time  $t$  if the chain starts from time  $-T$ ,  $W_t^{-T}$  is the number of individuals we are sure should be in the population at time  $t$ , and  $V_t^{-T}$  is the number of individuals for whom we are not sure whether they should be in the population at time  $t$  or not. We assume that we know nothing about the individuals in the population at time  $-T$ , so  $V_{-T}^{-T} = Y_{-T}$ , and  $W_{-T}^{-T} = 0$ . The construction of  $X_t^{-T}$  process will depend on the constructions of  $W_t^{-T}$  and  $V_t^{-T}$  which are shown as follows.

- At time  $-T$  set  $W_{-T}^{-T} = 0$ ,  $V_{-T}^{-T} = Y_{-T}$ .
- For  $t \in \mathcal{L}$ ,  
if  $t$  is a birth time of  $Y$ ,

$$\begin{aligned}
 W_t^{-T} &= W_{t^-}^{-T} + 1, V_t^{-T} = V_{t^-}^{-T}, & \text{if } p_t &\leq \frac{\min_{v \leq V_{t^-}^{-T}} \alpha(W_{t^-}^{-T} + v)}{\lambda}, \\
 W_t^{-T} &= W_{t^-}^{-T}, V_t^{-T} = V_{t^-}^{-T}, & \text{if } p_t &> \frac{\max_{v \leq V_{t^-}^{-T}} \alpha(W_{t^-}^{-T} + v)}{\lambda}, \\
 W_t^{-T} &= W_{t^-}^{-T}, V_t^{-T} = V_{t^-}^{-T} + 1, & \text{if } \frac{\min_{v \leq V_{t^-}^{-T}} \alpha(W_{t^-}^{-T} + v)}{\lambda} &< p_t \\
 & & &\leq \frac{\max_{v \leq V_{t^-}^{-T}} \alpha(W_{t^-}^{-T} + v)}{\lambda};
 \end{aligned}$$

if  $t$  is a death time of  $Y$ ,

$$\begin{aligned}
 W_t^{-T} &= W_{t^-}^{-T} - 1, V_t^{-T} = V_{t^-}^{-T}, & \text{if } p_t &\leq \frac{W_{t^-}^{-T}}{Y_{t^-}}, \\
 W_t^{-T} &= W_{t^-}^{-T}, V_t^{-T} = V_{t^-}^{-T}, & \text{if } p_t &> \frac{X_{t^-}^{-T}}{Y_{t^-}}, \\
 W_t^{-T} &= W_{t^-}^{-T}, V_t^{-T} = V_{t^-}^{-T} - 1, & \text{if } \frac{W_{t^-}^{-T}}{Y_{t^-}} &< p_t \leq \frac{X_{t^-}^{-T}}{Y_{t^-}}.
 \end{aligned}$$

- If  $V_0^{-T} = 0$  we output  $X_0^{-T} = W_0^{-T}$ . Otherwise we go back further in time and repeat the above procedure until  $V_0^{-T} = 0$ .

In the following we show the correctness of the above construction.

**Theorem 1.** *Suppose we simulate  $X$  with an initial value  $X_{-T}^{-T} = W_{-T}^{-T} + V_{-T}^{-T} = Y_{-T}$ . If there exists  $t_0 \in [-T, 0]$  such that  $V_{t_0}^{-T} = 0$ , then  $V_t^{-T} = 0$  for all*

$t \in [t_0, 0]$ . Furthermore, the process  $X_t^{-T} = W_t^{-T}$  for  $t > t_0$  evolves as a birth-death process defined by (1).

**Proof.** First note that for each fixed initial time  $-T$ , we can simulate  $X$  with an initial value  $X_{-T}^{-T} = Y_{-T}$  as follows.

If  $Y$  has a birth at  $t$  ( $Y_t = Y_{t-} + 1$ ), then  $X_t^{-T} = X_{t-}^{-T} + 1$  if  $p_t \leq \alpha(X_{t-}^{-T})/\lambda$ , and  $X_t^{-T} = X_{t-}^{-T}$  otherwise.

On the other hand, if  $Y$  has a death at  $t$  ( $Y_t = Y_{t-} - 1$ ), then  $X_t^{-T} = X_{t-}^{-T} - 1$  if  $p_t \leq X_{t-}^{-T}/Y_{t-}$ , and  $X_t^{-T} = X_{t-}^{-T}$  otherwise.

Kendall (1996) showed that the process  $X$  constructed above is a birth-death process defined by (1).

Now let us look at the non-monotone CFTP algorithm. Suppose  $V_{t_0}^{-T} = 0$  and  $t > t_0$  is the first jump time of  $X$  after  $t_0$ . Then  $V_t^{-T} = V_{t_0}^{-T} = 0$ ,  $X_t^{-T} = W_t^{-T}$ , and

$$\min_{v \leq V_t^{-T}} \alpha(W_t^{-T} + v) = \max_{v \leq V_t^{-T}} \alpha(W_t^{-T} + v) = \alpha(W_t^{-T}) = \alpha(X_t^{-T}).$$

So if  $t$  is a birth time of  $Y$ , then

$$W_t^{-T} = W_{t-}^{-T} + 1, V_t^{-T} = V_{t-}^{-T} = 0, \quad \text{if } p_t \leq \frac{\min_{v \leq V_{t-}^{-T}} \alpha(W_{t-}^{-T} + v)}{\lambda} = \frac{\alpha(X_{t-}^{-T})}{\lambda},$$

$$W_t^{-T} = W_{t-}^{-T}, \quad V_t^{-T} = V_{t-}^{-T} = 0, \quad \text{if } p_t > \frac{\max_{v \leq V_{t-}^{-T}} \alpha(W_{t-}^{-T} + v)}{\lambda} = \frac{\alpha(X_{t-}^{-T})}{\lambda},$$

and  $W_t^{-T} = W_{t-}^{-T}$ ,  $V_t^{-T} = V_{t-}^{-T} + 1$  will never happen for  $t > t_0$ . Therefore we have  $X_t^{-T} = W_t^{-T} + V_t^{-T} = W_t^{-T}$ .

On the other hand, if  $t$  is a death time of  $Y$ , then

$$W_t^{-T} = W_{t-}^{-T} - 1, V_t^{-T} = V_{t-}^{-T} = 0, \quad \text{if } p_t \leq \frac{W_{t-}^{-T}}{Y_{t-}} = \frac{X_{t-}^{-T}}{Y_{t-}},$$

$$W_t^{-T} = W_{t-}^{-T}, \quad V_t^{-T} = V_{t-}^{-T} = 0, \quad \text{if } p_t > \frac{X_{t-}^{-T}}{Y_{t-}},$$

and  $W_t^{-T} = W_{t-}^{-T}$ ,  $V_t^{-T} = V_{t-}^{-T} - 1$  will never happen for  $t > t_0$ . It is clear that, in any case, we have  $X_t^{-T} = W_t^{-T} + V_t^{-T} = W_t^{-T}$ . Therefore the process  $X_t^{-T} = W_t^{-T}$  for  $t > t_0$  is a birth-death process defined by (1). Furthermore,  $V_t^{-T} = 0$  for all  $t \in [t_0, 0]$  and, specifically, we have  $V_0^{-T} = 0$ .

It is noted that  $Y_t = 0$  will eventually occur for large enough  $T$ , so  $V_t^{-T} = 0$  will occur for large enough  $T$ . Furthermore, we have the following result.

**Theorem 2.** *Suppose  $Y_{t_0} = 0$  for some  $t_0 \in [-T, 0]$ . Then for any  $-S \leq -T \leq t_0 \leq t \leq 0$ , we have  $X_t^{-S} = X_t^{-T}$ .*

**Proof.** Since  $Y_{t_0} = 0$ , and  $X_{t_0}^{-T} = W_{t_0}^{-T} + V_{t_0}^{-T} \leq Y_{t_0}$ ,  $X_{t_0}^{-S} = W_{t_0}^{-S} + V_{t_0}^{-S} \leq Y_{t_0}$ , we see that  $W_{t_0}^{-S} = W_{t_0}^{-T} = 0$ ,  $V_{t_0}^{-S} = V_{t_0}^{-T} = 0$ ,  $X_{t_0}^{-S} = X_{t_0}^{-T} = 0$ . Therefore, any chains starting from any time  $-S \leq -T$  will coalesce at time  $t_0$ . Furthermore, it follows from Theorem 1 that for any  $t \in [t_0, 0]$ ,  $X_t^{-S} = X_t^{-T} = W_t^{-T}$ . This completes the proof.

Since we know that the process (1) converges to its equilibrium, it follows from Theorem 1 and Theorem 2 that the value of  $X_0^{-T} = W_0^{-T}$  is a perfect sample from this equilibrium distribution.

### 5. Area-interaction Point Processes

Consider an area-interaction point process in  $\mathcal{R}^d$  with distribution having a Radon-Nikodym density  $p(X)$  with respect to the unit rate Poisson process restricted to a compact window  $\mathcal{W}$ . Thus

$$p(X) = \alpha \lambda^{\#(X)} \gamma^{-m_d(X \oplus G)},$$

where  $\alpha$  is a normalization constant,  $\lambda, \gamma$  are positive parameters, and the grain  $G$  is a compact subset of  $\mathcal{R}^d$ ,  $X \oplus G = \bigcup \{x \oplus G : x \in X\}$ . The attractive case has  $\gamma > 1$ , while  $\gamma < 1$  corresponds to a repulsive case. We want to obtain a perfect sample from this point process.

#### 5.1. Monotone CFTP approach to area-interaction processes

Following Kendall's (1998) work, a dominant process can be constructed as a space-time Boolean model  $\Psi \subset \mathcal{W} \times \mathcal{R}$ :

$$\Psi = \bigcup \{(G \oplus x) \times [s, s + \ell] : [(x, s, \ell); p] \in Z\},$$

where  $Z$  is a Poisson process on  $\mathcal{R}^d \times \mathcal{R} \times (0, \infty) \times [0, 1]$  governed by the intensity measure

$$\left( \lambda e^{-\ell} \mathcal{I}_{[x \in \mathcal{W}]} \right) m_d(dx) m_1(ds) m_1(d\ell) m_1(dp).$$

Here  $s$  is called the birth time of the cylinder  $(G \oplus x) \times [s, s + \ell]$ , and  $s + \ell$  is called the death time of the cylinder. Furthermore for each  $(G \oplus x)$ , a mark  $p$  is attached with  $p$  chosen randomly in  $(0, 1)$ .

The basic idea of the dominated CFTP method for area-interaction point processes is to use the ordered list of space-time cylinder birth and death times lying in  $[-T, 0]$  in order to construct two time-evolving point processes  $Y^{\max}(-T, u)$ ,  $Y^{\min}(-T, u)$  on  $\mathcal{W} \subseteq \mathcal{R}^d$  such that  $Y(-T, u)$  will always be sandwiched between  $Y^{\max}(-T, u)$  and  $Y^{\min}(-T, u)$  for any  $-T \leq u \leq 0$ , these all have the common equilibrium distribution which is the distribution of the target area-interaction point process  $X$ .

Specifically let  $\mathcal{L}$  be the set of ordered list of space-time cylinder birth and death times lying in  $[-T, 0]$  and take

$$Z^{[-T,0]} = \{[(x, s, \ell); p] \in Z : -T \leq s + \ell, s \leq 0\},$$

$$\Xi(-T, t) = Y(-T, t-) \oplus G = \bigcup \{G \oplus x : x \in Y(-T, t-)\},$$

$$\Xi^{\min}(-T, t) = Y^{\min}(-T, t-) \oplus G, \Xi^{\max}(-T, t) = Y^{\max}(-T, t-) \oplus G.$$

Then the construction of a dominated CFTP for the area-interaction process when  $d = 2$  is given as follows.

- At time  $-T$  set

$$Y^{\max}(-T, -T) = \{x : [(x, s, l); p] \in Z^{[-T,0]}, s \leq -T \leq s+l\},$$

$$Y^{\min}(-T, -T) = \{x : [(x, s, l); p] \in Z^{[-T,0]}, s \leq -T \leq s+l, p \leq \gamma^{-m_2(G)}\}.$$

- For  $t \in \mathcal{L}$ ,

if  $t$  is a death time of a cylinder,

$$Y^{\min}(-T, t) = Y^{\min}(-T, t-) \setminus \{x\},$$

$$Y^{\max}(-T, t) = Y^{\max}(-T, t-) \setminus \{x\};$$

if  $t$  is a birth time of a cylinder and  $\gamma > 1$ ,

$$Y^{\min}(-T, t) = Y^{\min}(-T, t-) \cup \{x\} \quad \text{if } p \leq \gamma^{-m_2((G \oplus x) \setminus \Xi^{\min}(-T, t-))},$$

$$Y^{\max}(-T, t) = Y^{\max}(-T, t-) \cup \{x\} \quad \text{if } p \leq \gamma^{-m_2((G \oplus x) \setminus \Xi^{\max}(-T, t-))};$$

if  $t$  is a birth time of a cylinder and  $\gamma < 1$ ,

$$Y^{\min}(-T, t) = Y^{\min}(-T, t-) \cup \{x\} \quad \text{if } p \leq \gamma^{m_2(G) - m_2((G \oplus x) \setminus \Xi^{\max}(-T, t-))},$$

$$Y^{\max}(-T, t) = Y^{\max}(-T, t-) \cup \{x\} \quad \text{if } p \leq \gamma^{m_2(G) - m_2((G \oplus x) \setminus \Xi^{\min}(-T, t-))}.$$

- If  $Y^{\min}(-T, 0) = Y^{\max}(-T, 0)$  we output  $Y^{\min}(-T, 0)$ . Otherwise, we go back further in time and repeat the above procedure until coalescence occurs.

Kendall (1998) proved that the above algorithm terminates at finite time with probability one and the output is a perfect sample from the area-interaction point process.

**5.2. Non-monotone CFTP approach to area-interaction point processes**

From Kendall (1998) we see that the monotone property of the acceptance probability involved in the above construction is crucial. Without using this monotone structure, we need to explore a way of expressing the uncertainty at any time  $t$ .

It is noted that the state of the underlying Markov chain  $Y(-T, t)$  at time  $t$ , starting from time  $-T$ , is a point pattern in a bounded window  $\mathcal{W}$ . By using this fact we let

$$Y(-T, t) = W(-T, t) \cup V(-T, t),$$

where  $W(-T, t)$  is the part of  $Y(-T, t)$  which consists of all the points that should be in the point configuration  $Y(-T, t)$  at time  $t$ , and  $V(-T, t)$  is the part of  $Y(-T, t)$  which consists of all the points that may or may not be in the  $Y(-T, t)$  at time  $t$ . Furthermore, let all the points in  $W(-T, t)$  have an extra mark  $q = 0$  and all the points in  $V(-T, t)$  have an extra mark  $q = 1$ . Then when all the points in  $Y(-T, t)$  have marks  $q = 0$  we have a perfect sample from the equilibrium distribution. Specifically, a dominated non-monotone CFTP method for area-interaction point processes can be constructed as follows ( the construction of  $W(-T, t)$  and  $V(-T, t)$  are implicit).

- At time  $-T$ , set  $Y(-T, -T) = \{x : [(x, s, l); p] \in Z^{[-T, 0]}, s \leq -T \leq s + l\}$  and assign marks  $q = 1$  to all the points.

- For  $t \in \mathcal{L}$ ,

if  $t$  is a death time of a cylinder  $[(x, s, l) : p] \in Z$ ,  $Y(-T, t) = Y(-T, t-) \setminus \{x\}$ ;

**if  $t$  is a birth time of a cylinder and  $\gamma > 1$** , then if

$$p \leq \gamma^{-m_2((G \oplus x) \setminus \Xi(-T, t-))} \tag{3}$$

is independent of those points with  $q = 1$  and alive at time  $t-$ , we have  $Y(-T, t) = Y(-T, t-) \cup \{x\}$  and assign a mark  $q = 0$  to the new-born  $x$ , and if

$$p > \gamma^{-m_2((G \oplus x) \setminus \Xi(-T, t-))} \tag{4}$$

is independent of those points with  $q = 1$  and alive at time  $t-$ , we have  $Y(-T, t) = Y(-T, t-)$ . In any other cases we have  $Y(-T, t) = Y(-T, t-) \cup \{x\}$  and assign a mark  $q = 1$  to the new-born  $x$ .

**If  $t$  is a birth time of a cylinder and  $\gamma < 1$** , then if

$$p \leq \gamma^{m_2(G) - m_2((G \oplus x) \setminus \Xi(-T, t-))} \tag{5}$$

is independent of those points with  $q = 1$  and alive at time  $t-$ , we have  $Y(-T, t) = Y(-T, t-) \cup \{x\}$  and assign a mark  $q = 0$  to the new-born  $x$ , and if

$$p > \gamma^{m_2(G) - m_2((G \oplus x) \setminus \Xi(-T, t-))} \quad (6)$$

is independent of those points with  $q = 1$  and alive at time  $t-$ , we have  $Y(-T, t) = Y(-T, t-)$ . In any other cases we have  $Y(-T, t) = Y(-T, t-) \cup \{x\}$  and assign a mark  $q = 1$  to the new-born  $x$ .

- If all the points in  $Y(-T, 0)$  have a mark  $q = 0$ , we output  $Y(-T, 0)$ . Otherwise, we go back further in time and repeat the above procedure until  $q = 0$  for all the points in  $Y(-T, 0)$ .

Note that conditions (3), (4), (5) and (6) are easy to check since only those grains which overlap with the new born grain are involved. Comparing with the dominated monotone CFTP for the area interaction point processes, we see that

- All points which are accepted with  $q = 0$  are those which should be accepted by both maximal and minimal processes at time  $t$ .
- All points which are accepted with  $q = 1$  are those which should be accepted only by the maximal process.
- All points which are rejected are those which should be rejected by both maximal and minimal processes.

Therefore, once all the points in the pattern by time  $t = 0$  have  $q = 0$ , the maximal and minimal processes coalesce and we have a perfect sample.

### 5.3. The performance of the algorithm and examples

For each run the program terminates once a perfect sample is obtained. The running time depends on the values of  $\lambda$ ,  $\gamma$  and the radius of the grain  $r$ , etc. The relationship between them is complicated. In the following, we consider several special cases. In all cases, the length of the observed window  $\mathcal{W}$  is 10, the initial time interval is  $[-2, 0]$ . All the results are obtained by running the program on a COMPAQ Laptop (Pentium II, 64 MB memory).

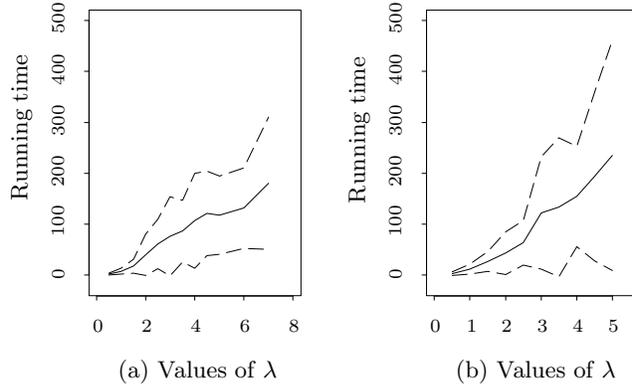
#### (A) Relationship between running time and the values of $\lambda$ .

In the attractive case, we let  $\ln \gamma = 2$ ,  $r = 0.5$ ,  $\lambda = 0.1, 0.5, 1, 1.5, \dots, 4.5, 5, 6, 7$ .

In the repulsive case, we let  $\ln \gamma = -2$ ,  $r = 0.5$ ,  $\lambda = 0.1, 0.5, 1, 1.5, \dots, 4.5, 5$ .

For each value of  $\lambda$ , we ran the corresponding program 50 times. Each time we started with a different random seed for the random number generator. After each run we recorded the CPU time. Therefore, for each  $\lambda$ , we have 50 recorded running times. By working out the sample mean  $\bar{x}_\lambda$  and the sample standard

deviation  $s_\lambda$  of the running time, we obtained Figure 1. In Figure 1 the solid curves are the sample means, the two dash curves are the curves of  $\bar{x}_\lambda \pm 2s_\lambda$ .



(a) Attractive case with  $\ln \gamma = 2$ ,  $r = 0.5$  and  $\lambda = 0.1, 0.5, 1, 1.5, \dots, 4.5, 5, 6, 7$ .  
 (b) Repulsive case with  $\ln \gamma = -2$ ,  $r = 0.5$ , and  $\lambda = 0.1, 0.5, 1, 1.5, \dots, 4.5, 5$ .

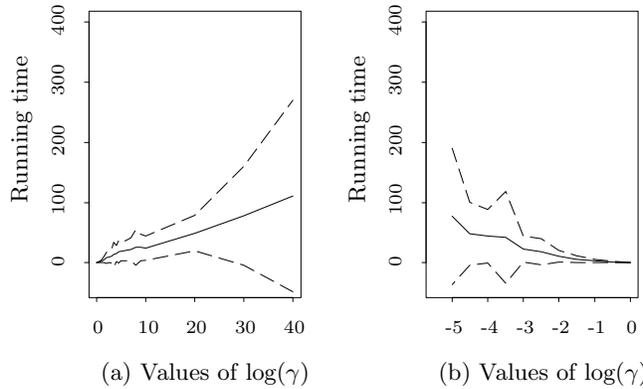
Figure 1. Running time (in seconds) versus the values of  $\lambda$ .

**(B) Relationship between running time and the value of  $\gamma$ .**

In the attractive case, we let  $\lambda = 1$ ,  $r = 0.5$ ,  $\ln \gamma = 0, 0.5, 1.5, \dots, 4.5, 5, 6, 7, 8, 9, 10, 20, 30, 40$ .

In the repulsive case, we let  $\lambda = 1$ ,  $r = 0.5$ ,  $\ln \gamma = 0, -0.5, -1.5, \dots, -4.5, -5$ .

As in **(A)**, for each value of  $\ln \gamma$  we ran the corresponding program 50 times and recorded the running time. The results are shown in Figure 2.



(a) Attractive case with  $\lambda = 1$ ,  $r = 0.5$ , and  $\ln \gamma = 0, 0.5, 1.5, \dots, 4.5, 5, 6, 7, 8, 9, 10, 20, 30, 40$ .  
 (b) Repulsive case with  $\lambda = 1$ ,  $r = 0.5$  and  $\ln \gamma = 0, -0.5, -1.5, \dots, -4.5, -5$ .

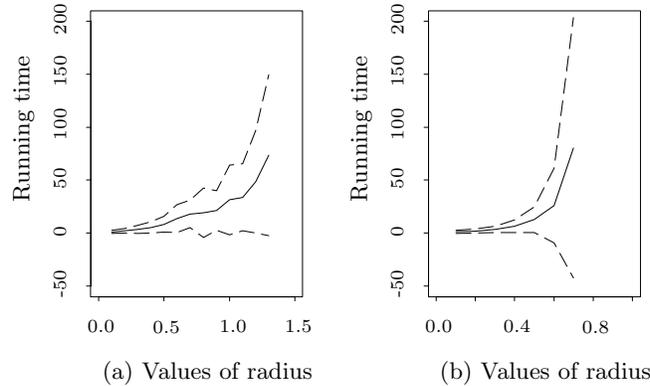
Figure 2. Running time (in seconds) versus the values of  $\ln \gamma$ .

**(C) Relationship between running time and the values of  $r$ .**

In the attractive case, we let  $\lambda = 1$ ,  $\ln \gamma = 2$ , and  $r = 0.1, 0.2, \dots, 1.2, 1.3$ .

In the repulsive case, we let  $\lambda = 1$ ,  $\ln \gamma = -2$ , and  $r = 0.1, 0.2, \dots, 0.7$ .

Again, as in (A), for each value of  $r$  we ran the corresponding program 50 times and recorded the running time. The results are shown in Figure 3



(a) Attractive case with  $\lambda = 1$ ,  $\ln \gamma = 2$ , and  $r = 0.1, 0.2, \dots, 1.2, 1.3$ .  
 (b) Repulsive case with  $\lambda = 1$ ,  $\ln \gamma = -2$ , and  $r = 0.1, 0.2, \dots, 0.7$ .

Figure 3. Running time (in seconds) versus the values of  $r$ .

There are several common features in Figures 1, 2 and 3. First, as values of the parameters increase (or  $\gamma$  decreases in the repulsive case) the running time also increases. This is what was expected, because in this case the interaction between points becomes stronger when the number of points in a fixed window  $\mathcal{W}$  increases, when the value of  $\gamma$  changes, which itself measures the level of interaction in some way, and when the radius of the grain increases so that more and more grains overlap with each other.

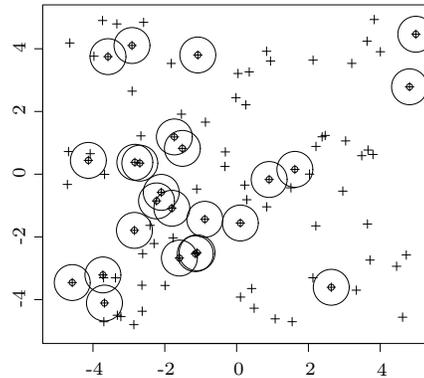
Second, on average, the repulsive case program is slower than the attractive one, especially when the absolute values of the parameters become large. However we would like to comment that this is true only for the specific values of the parameters we have chosen. Indeed when we checked the running times, we found that for the parameter values  $\lambda = 1$ ,  $\ln \gamma = 2$  and  $r = 0.5$  in the attractive case,  $\lambda = 1$ ,  $\ln \gamma = -2$  and  $r = 0.5$  in the repulsive case, on average, the repulsive case program is faster than the attractive one. The region of triples  $(\lambda, \gamma, r)$  for which the attractive case method is faster than the repulsive case needs further investigation.

Third, the variations of the running time increase as the values of the parameters increase (or  $\gamma$  decreases in the repulsive case). A possible explanation

is as follows. The stronger the interaction between points, the longer running time is required. The longer running time increases the chances of getting an “extreme” point pattern during the simulation and this needs longer running time for coalescence. Consequently, the variability of the running time increases.

Next we show two perfect samples from an area-interaction point processes. The parameters are set as follows.

For the attractive area-interaction point process, we let  $\lambda = 1$ ,  $\gamma = e^2 = 7.39$ , the length of the window  $\mathcal{W}$  be 10, the radius of the grain be 0.5, and the initial time interval be  $[-2, 0]$ . We run the attractive program on the above setting and get the results shown in Figure 4.

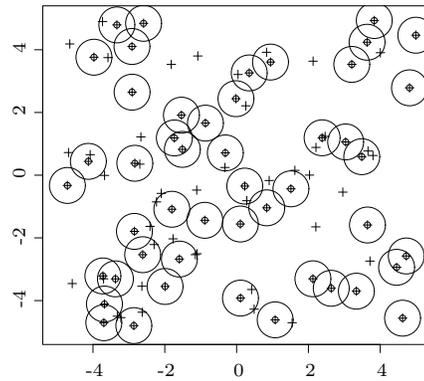


Perfect sample from an attractive area-interaction point process with  $\lambda = 1$ ,  $\gamma = e^2 = 7.39$ , the length of the window is 10, the radius of the grain is 0.5 and the initial time interval is  $[-2, 0]$ . In the figure, the cross points are those in the initial pattern, the cross-circle points are those in the final perfect sample.

Figure 4. A perfect sample from an attractive area-interaction point process.

For the repulsive area-interaction point process, we let  $\lambda = 1$ ,  $\gamma = e^{-2} = 0.135$ , the length of the window  $\mathcal{W}$  be 10, the radius of the grain be 0.5, and the initial time interval be  $[-2, 0]$ . We run the repulsive program on the above setting and get the results shown in Figure 5.

Note that we use the same initial Poisson point pattern in the observed window  $\mathcal{W}$  for both examples. From Figure 4 and Figure 5 we see that the union of grains of the final sample from the attractive area-interaction point process covers less area of the window  $\mathcal{W}$  than that from the repulsive area-interactive point process. Especially, it is worth mention that the attractive point process tends to accept those points which are close together, while the repulsive point process tends to reject them. This is as expected.



Perfect sample from a repulsive area-interaction point process with  $\lambda = 1$ ,  $\gamma = e^{-2} = 0.135$ , the length of the window is 10, the radius of the grain is 0.5, and the initial time interval is  $[-2, 0]$ . In the figure, the cross points are those in the initial pattern, the cross-circle points are those in the final perfect sample.

Figure 5. A perfect sample from a repulsive area-interaction point process.

## 6. Conclusions and Comments

We have presented a non-monotone CFTP method. We applied the new method to a general birth-death process and to attractive/repulsive area-interaction point processes.

If the uncertainty at any time  $t$  can be expressed by the difference between maximum and minimum states according to some monotone structure, then the method presented in this paper is similar to the corresponding monotone CFTP method which has been shown through area-interaction point processes. However, if there exists no monotone structure, the method presented in this paper will work. Moreover, the new method needs less computer memory since only one chain needs to be run.

Finally we point out that it is possible to construct a dominated non-monotone CFTP algorithm for conditional Boolean models (Kendall and Thönnies (1999)) and for correlated Poisson random variables conditioned to be positive (Cai and Kendall (2002)).

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