

Perfect simulation for a stationary silo with absorbing walls

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Abstract The objective of this work is to generate random samples of the unique stationary distribution associated to the stochastic model for grain storage in a finite bidimensional silo. The support of this measure is an unbounded and continuous state space and therefore a truncation was necessary to apply the CFTP perfect simulation scheme. The performance of the algorithm was measured by comparing the sample moments to the theoretical ones.

Key words: CFTP, invariant measure, granular media

AMS Classification: Primary: 65C40,60K35; Secondary:82C20, 82C22

1 Introduction

In the nearest neighbors one dimensional uniform q-model of force fluctuations in bead packs each grain is thought as having weight 1 and supporting the weight of the grains of higher layers. This weight is distributed between the two neighboring grains of the following lower layer in the silo according to uniform distribution.

To define the model let $(U_t) := \{U_t(i) : i \in \mathbb{Z}, t \geq 0\}$ be a family of independent uniform random variables in $[0, 1]$ and $(V_t) := \{V_t(i) : i \in \mathbb{Z}, t \geq 0\}$ be a family of iid positive random variables with mean 1 and variance $S = \mathbb{V}V_t(i)$. Furthermore assume (V_t) and (U_t) to be independent families.

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Fix $N \geq 1$, consider the finite box

$$\Lambda^N := \{1, \dots, N\}$$

and denote $W_t^N(i)$ the weight carried by a grain located at the i th position at level t . Fix an initial configuration $W_0^N \in [0, \infty)^N$ and define inductively

$$\begin{aligned} W_t^N(i) &= V_t(i) + W_{t-1}^N(i+1)U_{t-1}(i+1) + W_{t-1}^N(i-1)(1 - U_{t-1}(i-1)), \quad \text{for } i \in \Lambda^N \\ W_t^N(0) &= W_t^N(N+1) \equiv 0 \end{aligned} \tag{1.1}$$

Let $(W_t) = (W_t(i) : i \in \Lambda^N)$; then $(W_t^N : t \geq 1)$ is a discrete time Markov chain on $\mathcal{S} := [0, \infty)^N$. Each grain j of layer t gives a fraction chosen uniformly in $[0, 1]$ of its own weight plus the total weight it supports from the previous layers to grain $j - 1$ of the successive layer $t + 1$ (which we can think is below t) and the remaining to grain $j + 1$. The weight distributed to grains outside Λ^N is thought of as being absorbed by the walls of the silo at sites 0 and $N + 1$. Denote $\nu S^N(t)$ the measure defined by

$$\nu S^N(t)f = \int \nu(dW) \mathbb{E}(f(W_t^N) | W_0^N = W).$$

where \mathbb{E} and \mathbb{P} are the expectation and probability defined with respect to the probability space induced by $(U_t : t \geq 0)$ and $(V_t : t \geq 0)$.

We say that a measure μ^N is *invariant* for the process W_t^N if $\mu^N S^N(t) = \mu^N$.

If W_t^N has an invariant measure μ^N its mean heights $w^N(i) := \mu^N(W^N(i))$ have to satisfy the following system of equations (coming from $\mu^N S^N(t)W^N(i) = \mu^N W^N(i)$):

$$\begin{aligned} w^N(i) &= 1 + \frac{1}{2}w^N(i-1) + \frac{1}{2}w^N(i+1), \quad \text{for } i \in \Lambda^N; \\ w^N(i) &= 0, \quad \text{for } i \in \mathbb{Z} \setminus \Lambda^N. \end{aligned} \tag{1.2}$$

Notice that $w^N(i)$ has quadratic profile:

$$w^N(i) = i(N+1-i), \quad \text{for } i = 0, \dots, N+1. \tag{1.3}$$

(It is the expected time to exit Λ^N for a symmetric nearest neighbor random walk starting at i .)

Denote the covariance matrix by

$$\sigma^N(i, j) := \text{Cov}_{\mu^N}[W^N(i), W^N(j)].$$

If W_0^N is distributed according to the invariant measure, so is W_1^N , and one can use (1.1) to show that $\sigma^N(i, j)$ satisfies the system of equations:

$$\begin{aligned}
\sigma^N(i, i) &= S + \frac{1}{3}\sigma^N(i+1, i+1) + \frac{1}{3}\sigma^N(i-1, i-1) + \frac{1}{4}\sigma^N(i-1, i+1) \\
&\quad + \frac{1}{4}\sigma^N(i+1, i-1) + \frac{1}{12}(w^N(i+1))^2 + \frac{1}{12}(w^N(i-1))^2, \quad i \in \Lambda^N \\
\sigma^N(i, i+2) &= \frac{1}{4}\sigma^N(i+1, i+3) + \frac{1}{4}\sigma^N(i-1, i+3) + \frac{1}{4}\sigma^N(i-1, i+1) \\
&\quad + \frac{1}{6}\sigma^N(i+1, i+1) - \frac{1}{12}(w^N(i+1))^2, \quad i \in \{1, \dots, N-2\} \\
\sigma^N(i, i-2) &= \frac{1}{4}\sigma^N(i+1, i-1) + \frac{1}{4}\sigma^N(i-1, i-3) + \frac{1}{4}\sigma^N(i+1, i-3) \\
&\quad + \frac{1}{6}\sigma^N(i-1, i-1) - \frac{1}{12}(w^N(i-1))^2, \quad i \in \{3, \dots, N\} \\
\sigma^N(i, j) &= \frac{1}{4}\sigma^N(i+1, j+1) + \frac{1}{4}\sigma^N(i-1, j-1) + \frac{1}{4}\sigma^N(i-1, j+1) \\
&\quad + \frac{1}{4}\sigma^N(i+1, j-1), \quad i, j \in \Lambda^N, \quad |i-j| \geq 2 \\
\sigma^N(i, j) &= 0, \quad i \in \{0, N+1\} \text{ or } j \in \{0, N+1\}.
\end{aligned} \tag{1.4}$$

The above model in which a grain lies its weight onto the lower neighbors was introduced by Harr (1977) and explored by others, for example, Liu, Nagel, Schecter, Coppersmith, Majumdar, Narayan and Witten (1995) introduced the model defined by (1.1). The model with zero boundary condition was studied by Peralta-Fabi, Málaga and Rechtman (1997). Barros, Ferrari, Garcia and Martínez (2001) show the existence and uniqueness of the invariant measure. To show uniqueness they couple two versions of the process starting with different initial invariant distributions using the same sequence U_t for both evolutions. However, there is no explicit formula for the invariant measure and to obtain a random sample from this measure we have to resort to stochastic simulation.

Usually Monte Carlo Markov Chain methods have been used to generate samples from probability distributions that are not known explicitly. The most common approach is to identify this distribution as the invariant measure of a Markov chain and run the corresponding chain for a long time until its distribution is close to equilibrium. The problem here is to assess how long the chain should run in order to achieve the desired approximation. In finite state Markov chains, this is related to mixing times and cut-off phenomena [see, Aldous and Fill (1999)]. For uncountable state space, more specifically for continuous unbounded state spaces these techniques are not applied. However, after

the pioneer work of Propp and Wilson (1996) we can reach a much more ambitious goal: to simulate perfectly from the invariant distribution. *Perfect simulations* or *exact sampling* are labels for a recently developed set of techniques designed to produce output whose distribution is guaranteed to follow a given probability law. These techniques are particularly useful in relation with Markov Chain Monte Carlo, and their range of applicability is rapidly growing (see Green and Murdoch (1999), Section 1.3, and Mira, Møller and Roberts (1999) and Møller and Nicholls (1999) and references therein, or visit the site <http://dimacs.rutgers.edu/~dbwilson/exact>).

The outbreak of these subject come with Propp and Wilson (1996) paper where they suggest a practical method of achieving a perfect sample of a Markov chain with finite state space. Their *Coupling from the Past* (CFTP) algorithm have also been applied for infinite (or huge) state spaces requiring a *monotonicity property*: there must exist a “maximal” and a “minimal” state and a coupling such that the coalescence of trajectories starting from these two states imply the coalescence of all other trajectories (“monotone coupling”). In the case of unbounded infinite (or very large) state space, it is not possible to use the above described method. Kendall (1998) introduced a modification in Propp and Wilson’s algorithm in order to apply it to some unbounded processes (Green and Murdoch, 1999). It is also called horizontal CFTP (Kendall and Møller, 1999) and coupling into and from the past (Wilson, 2000). The idea is to find another Markov chain $\{C_t, t \in \mathbb{Z}\}$ — chosen in such way that we know how to generate exactly from its invariant measure — that dominates the chain under study. When there is no domination for the process, as in the case of the silo model, there is no canonical solution and none of the perfect simulation schemes can be applied directly. The proposal of this work is to truncate the initial state and compare the so-called perfect sample obtained in this way with the stationary distribution through its first and second moment. This paper is organized as follows: In Section 2, a brief description of CFTP and dominated CFTP is given as well as the algorithms used for the silo model, Section 3 presents the simulation results.

2 Perfect simulation

2.1 CFTP

Let X_n be an ergodic discrete time Markov chain with finite state space \mathcal{S} , transition matrix $(P_{i,j})$ and invariant distribution π . Perfect simulation can be described as a procedure that provides an unbiased observation of π through some random mechanism.

One way of obtaining a perfect simulation is described by Propp and Wilson (1996) as *coupling from the past*. This approach can be described briefly as follows: simulate the Markov chain, coupling all the paths beginning from all possible initial states, a predetermined amount of time (from $-T$ to 0), if all paths coalesce at time 0, the coalescent state X_0 has the desired distribution π . If the paths did not coalesce, restart the chain at $-T' < -T$, from all possible initial states, preappending new moves to the old ones. They show that if enough moves are preappended, eventually all the paths will coalesce and the resulting coalescent state X_0 is an unbiased sample from π .

When the cardinality of the state space is very large, the above argument is not feasible. However for cases where there is a partial ordering in the state space, a maximal ($\hat{1}$) and a minimal state ($\hat{0}$) and moreover, the update of the chain is ordering preserving, then only two paths need to be simulated and coupling from the past can be used. The procedure can be described by the following pseudo-code:

```
 $T \leftarrow 1$   
 $U_{-1} \sim U(0,1)$   
repeat  
   $upper \leftarrow \hat{1}$   
   $lower \leftarrow \hat{0}$   
  for  $n = -T$  to  $-1$   
     $upper \leftarrow \phi(upper, U_n)$   
     $lower \leftarrow \phi(lower, U_n)$   
 $T \leftarrow 2T$   
for  $n = -T$  to  $-T/2$   
   $U_n \sim U(0,1)$ 
```

```

until upper = lower
return upper

```

Notice that the same uniform random variables are used for all loops, for instance, U_{-1} is going to be generated only once.

In the case of unbounded infinite (or very large) state space, it is not possible to use the above described method. Kendall (1998) introduced a modification in Propp and Wilson’s algorithm in order to apply it to point processes. The idea, however, is not limited to this case and has been used to generate from continuous unbounded state space (Green and Murdoch, 1999). It is also called horizontal CFTP (Kendall and Møller, 1999) and coupling into and from the past (Wilson, 2000).

The idea is to find another Markov chain $\{C_t, t \in \mathbb{Z}\}$ — chosen in such way that we know how to generate exactly from its invariant measure — that dominates the chain under study. If we have: (a) a coupling that guarantees that if for some t we have $C_t \geq X_t$ that the same is true for all subsequent times; (b) for any value $x \in \mathcal{S}$ and time $t < 0$, there exists a.s. an $s < t$ such that $X_t \leq C_t$ if $X_u = x$ for $u < s$; (c) we can simulate directly from the invariant distribution of C_t ; and (d) given C_t the conditional distribution of (C_{t-1}, U_{t-1}) is known and we can sample from this distribution. In this case, we can use the CFTP algorithm based on generating an upper process in the same way that vertical CFTP.

3 Perfect simulation of the stationary measure of the silo model

The purpose of this work is to perfect simulate a sample from the invariant measure for the Markov process given by (1.1) which has as its support the set $\mathcal{S} = [0, \infty)^N$ and there is no maximal state. Moreover, the only available information about this distribution is the first and second moments and it is not possible to find a chain that dominates the process in order to apply dominated CFTP. The suggested approach in this work is to use as an initial “maximal” state $[0, K]^N$ for K sufficiently large and generate a random sample from a new distribution ν_K . The goal is to find K big enough so that the distance between ν and ν_K is small enough.

3.1 Truncation error

Consider the process W_t defined by (1.1) and let

$$\nu(A) = \mathbb{P}(W_0 \in A, W_{-T(K)} \in [0, K]^N | W_{-\infty} = x) \quad (3.1)$$

$$\begin{aligned} &+ \mathbb{P}(W_0 \in A, W_{-T(K)} \notin [0, K]^N | W_{-\infty} = x) \\ &= \nu_K(A) \times \nu(W_{-T(K)} \in [0, K]^N). \end{aligned} \quad (3.2)$$

Notice that

$$\begin{aligned} 1 - \nu(W_{-T(K)}(x) \in [0, K]^N) &= \mathbb{P}_\nu(W_{-T(K)}(x) > K, \text{ for some } x = 1, \dots, N) \\ &\leq \sum_{x=1}^N \mathbb{P}_\nu(W_{-T(K)}(x) > K) \\ &\leq \sum_{x=1}^N \frac{\mathbb{E}_\nu[W_{-T(K)}(x)]}{K} \\ &= \sum_{x=1}^N \frac{x(N+1-x)}{K}, \end{aligned}$$

since $\mathbb{E}_\nu[W_{-T(K)}(x)] = x(N+1-x)$ by (1.3). Thus, for any $\delta > 0$ we can choose K big enough such that

$$\sum_{x=1}^N \frac{x(N+1-x)}{K} < \delta,$$

and consequently,

$$\begin{aligned} \mathbb{P}(W_0 \in A, W_{-T(K)} \notin [0, K]^N | W_{-\infty} = x) &\leq \mathbb{P}(W_{-T(K)} \notin [0, K]^N | W_{-\infty} = x) \\ &\leq \delta. \end{aligned}$$

Therefore, we can make the total variation distance $\|\nu(A) - \nu_K(A)\|$ as small as we wish by taking K sufficiently large,

$$\begin{aligned} \|\nu(A) - \nu_K(A)\| &= \sup_A |\nu_K(A)[\nu(W_{-T(K)} \in [0, K]^N) - 1] \\ &\quad + \mathbb{P}(W_0 \in A, W_{-T(K)} \notin [0, K]^N | W_{-\infty} = x)| \\ &\leq \sup_A |\nu_K(A)[1 - \nu(W_{-T(K)} \in [0, K]^N)]| \end{aligned}$$

$$\begin{aligned}
& + \sup_A |\mathbb{P}(W_0 \in A, W_{-T(K)} \notin [0, K]^N | W_{-\infty} = x)| \\
& = \sup_A |\nu_K(A)| \times |[1 - \nu(W_{-T(K)} \in [0, K]^N)]| \\
& + \sup_A |\mathbb{P}(W_0 \in A, W_{-T(K)} \notin [0, K]^N | W_{-\infty} = x)| \\
& \leq 2\delta.
\end{aligned} \tag{3.3}$$

3.2 CFTP applied to the silo model

Let \mathbb{M}_N be the space of $N \times N$ square matrices with elements belonging to $[0, 1]$. Define $\phi : [0, \infty)^N \times \mathbb{M}_N \rightarrow [0, \infty)^N$ by

$$\phi(W, \mathbb{U}) = \mathbb{1} + \mathbb{U}W,$$

with $\mathbb{1} = (1, \dots, 1)'$. Denote $W_t = (W_t(1), \dots, W_t(N))'$ and \mathbb{U}_t an $N \times N$ tridiagonal matrix such that, for

$$\mathbb{U}_t(i, j) = \begin{cases} U_t(j), & \text{if } j = i + 1 \\ 1 - U_t(j - 1), & \text{if } j = i - 1 \\ 0, & \text{otherwise} \end{cases} \tag{3.4}$$

where $\{\{U_t(j), j = 1, \dots, N\}, t = 0, 1, \dots\}$ is a family of i.i.d. $U(0, 1)$ random variables. The silo model can be rewritten in the matricial form as

$$\begin{aligned}
W_t & = \mathbb{1} + \mathbb{U}_{t-1}W_{t-1} \\
& = \phi(W_{t-1}, \mathbb{U}_{t-1}).
\end{aligned} \tag{3.5}$$

Consider the initial time to be $t = -L$, then and $W_{-L}^{(i)} = i$, then

$$\begin{aligned}
W_0 & = \phi_{-1}(\phi_{-2}(\phi_{-3}(\dots, \phi_{-L+1}(\phi_{-L}(W_{-L}^{(i)}, \mathbb{U}_{-L}), \mathbb{U}_{-L+1}), \dots, \mathbb{U}_{-3}), \mathbb{U}_{-2}), \mathbb{U}_{-1}) \\
& = \mathbb{1} + \mathbb{U}_{-1}\mathbb{1} + \mathbb{U}_{-1}\mathbb{U}_{-2}\mathbb{1} + \mathbb{U}_{-1}\mathbb{U}_{-2}\mathbb{U}_{-3}\mathbb{1} + \dots + \mathbb{U}_{-1}\mathbb{U}_{-2}\mathbb{U}_{-3}\dots\mathbb{U}_{-L+1}\mathbb{1} + \\
& \quad \mathbb{U}_{-1}\mathbb{U}_{-2}\mathbb{U}_{-3}\dots\mathbb{U}_{-L}W_{-L}^{(i)}.
\end{aligned} \tag{3.6}$$

Pseudo-algorithm: Define $\hat{0} = (0, \dots, 0)'$ and $\hat{1} = (K, \dots, K)'$ (K is going to be defined latter for each N in order to control the error given by (3.3)), to be the minimal and maximal state, respectively. Therefore, using the same uniform random variables to update both processes, the system is attractive and if $W_0^{(\hat{0})}(x) \leq W_0^{(\hat{1})}(x)$ for $x \in \{1, \dots, N\}$, then $W_t^{(\hat{0})}(x) \leq W_t^{(\hat{1})}(x)$ for all $x \in \{1, \dots, N\}$ and $t \geq 1$.


```

    t ← 0
    A ← (0, ..., 0)'1×N
    1 ← (1, ..., 1)'1×N
    V ← IN (IN = identity matrix of order N)
Repeat
    t ← t - 1
    Wt(0̂) ← 0̂
    Wt(1̂) ← 1̂
    Generate Ut
    V ← V × Ut
    W0(0̂) ← 1 + A + V × Wt(0̂)
    W0(1̂) ← 1 + A + V × Wt(1̂)
    A ← A + V × 1
Until || W0(1̂) - W0(0̂) ||∞ < ε.

```

The function $\| \cdot \|_{\infty}$ is the sup norm. In the simulation procedures $\epsilon = 10^{-5}$.

4 Simulation results

We simulate $m = 100$ samples of size $n = 50$ for each silo size $N = 5, 15, 21$. The truncation error was fixed to be around 3%, the truncation constants were computed using (3.3) (see Table 4.2). We represent each sample of size n by

$$\{W^{(1,i)}, \dots, W^{(n,i)}\}, \text{ for } i = 1, \dots, m. \quad (4.1)$$

Notice that each column is an iid random vector with distribution ν_K , with mean μ and covariance matrix Σ . Therefore, we can apply the multivariate central limit theorem to test if the mean and variance of the generated sample coincides with the theoretical results given by (1.3) and (1.4) respectively. For $i = 1, \dots, m$, define

$$\overline{W}^{(i)} = \frac{W^{(1,i)} + \dots + W^{(n,i)}}{n}. \quad (4.2)$$

We want to test the following hypothesis:

$$H_0 : \mu = w^N \times H_1 : \mu \neq w^N, \quad (4.3)$$

where w^N is given by (1.3). The appropriate test statistics to be used are:

$$T^2 = m(\overline{W} - w^N)'S^{-1}(\overline{W} - w^N),$$

where

$$\overline{W} = \frac{\overline{W}^{(1)} + \dots + \overline{W}^{(m)}}{m}$$

and

$$S^2 = \frac{1}{m-1} \sum_{j=1}^m (\overline{W}^{(j)} - \overline{W})(\overline{W}^{(j)} - \overline{W})'.$$

The sample statistics T^2 has asymptotic distribution given by $\frac{(m-1)N}{(m-N)} F_{N,m-N}$, where $F_{N,m-N}$ denotes the F -distribution with N and $(m-N)$ degrees of freedom.

In order to test the equality of the covariance matrix, we want to test

$$H'_0 : \Sigma = \Sigma^N/n \times H'_1 : \Sigma \neq \Sigma^N/n, \quad (4.4)$$

where $\Sigma^N(i, j)$ is given by system (1.4) and the likelihood ratio test was used. The test statistic is given by

$$\Lambda = \frac{\sup_{\mu} L(\mu, \Sigma^N)}{\sup_{\mu, \Sigma} L(\mu, \Sigma)}, \quad (4.5)$$

where

$$L(\mu, \Sigma) = (\det \Sigma)^{-m/2} \exp(\text{trace}(-1/2 \Sigma^{-1} A)) \exp[-1/2 m (\overline{W} - \mu)' \Sigma^{-1} (\overline{W} - \mu)].$$

In the last expression, $A = mS^2$. The numerator and denominator in (4.5) are easily determined by taking $\mu = \overline{W}$ and $\mu = \overline{W}$ e $\Sigma = \frac{A}{m}$, respectively.

The critical region for this test is of the form $-2 \log \Lambda \leq c$ with c chosen to guarantee the size of the test to be 0.05. The distribution of $-2 \log \Lambda$, under the null hypothesis is described by Muirhead (1946).

4.1 Numerical results

Figures 4.1 through 4.2 show that the sample mean is very close to the theoretical mean with quadratic profile. Table 4.1 shows the significance values (p-values) for the hypothesis testing, we can see that we do not have evidence to reject the hypothesis of equality of means and variance.

Table 4.1: p-values for the hypothesis testing of equality of means and equality of covariances

N	$\frac{(m-N)}{[(m-1)N]} T^2$	p-value (means)	$-2 \log \Lambda$	p-value (covariances)
5	1.14	0.34	21.05	0.876
15	1.23	0.27	137.6	0.877
21	1.05	0.41	235.6	0.584

4.2 Coalescence times

In order to study the distribution of the coalescence time, histograms were used (see Figures 4.4 through 4.6), in this case it seems reasonable to consider that the coalescence time follows a normal distribution. Table 4.2 presents the confidence interval for the mean coalescence time considering the normal approximation.

Table 4.2: Confidence interval for the mean coalescence time ($\mathbb{E}[T(K)]$), considering a truncation for the initial state space to be $[0, K]$

N	K	$\mathbb{E}[T(K)]$	S	CI(95%)
5	10.000	140.2	12	(139.89; 140.55)
15	30.000	1160.4	54.5	(1159.9; 1161.9)
21	50.000	2268.7	87.5	(2266.25; 2271.11)

Figure 4.1: Average sample weight and mean weight for silo of size $N = 5$

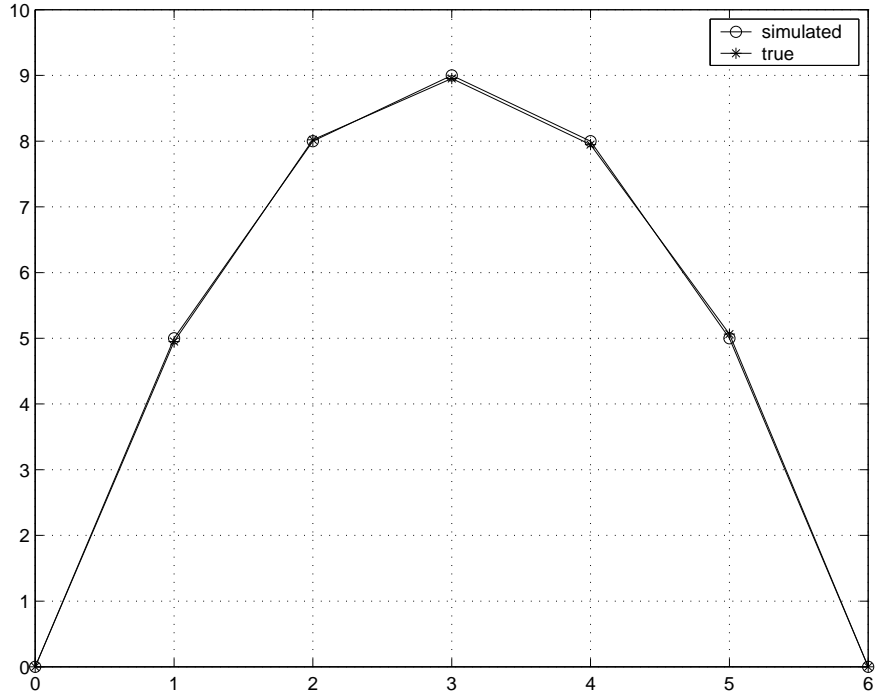
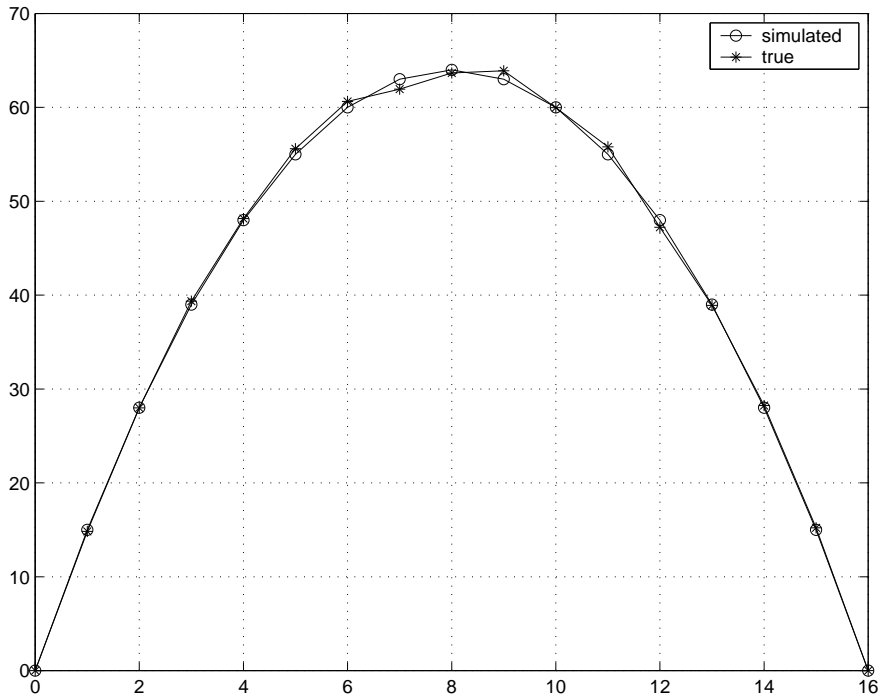


Figure 4.2: Average sample weight and mean weight for silo of size $N = 15$



4.2.1 Coalescence time as a function of silo width (N)

In order to empirically verify the relationship between coalescence time $T(K)$ and silo width N we generate for each size N , one sample with corresponding coalescence time $T(K)$. Table 4.3 show the coalescence times for several sizes.

Table 4.3: Coalescence time ($T(K)$)

N	$T(K)$	N	$T(K)$
5	132	115	82328
15	1233	125	95160
25	3524	135	112647
35	6978	145	135361
45	11353	155	152432
55	16760	165	172733
65	24382	175	196077
75	33157	185	221404
85	44529	195	246185
95	55541	205	271789
105	65801		

It seems that there exists an exponential relationship between the coalescence time and the size of the silo. Adjusting a linear regression we find that a good estimate for the model ($R^2 = 0.9974$) is

$$\log(\hat{T}(K)) = 1.96 \log(N) + 1.82. \quad (4.6)$$

MCMC methods could also be used to sample from an approximate distribution. However, only the first two moments are available for the true distribution ν . From the sample generated by truncated CFTP, there is equality of the first two moments of ν and ν_K and MCMC samples cannot do better. Furthermore, to perfectly simulate from an approximate distribution ν_K has the advantage that we can choose K in order to control the error and we do have a stopping rule which is not possible for any MCMC scheme.

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Figure 4.3: Average sample weight and mean weight for silo of size $N = 21$

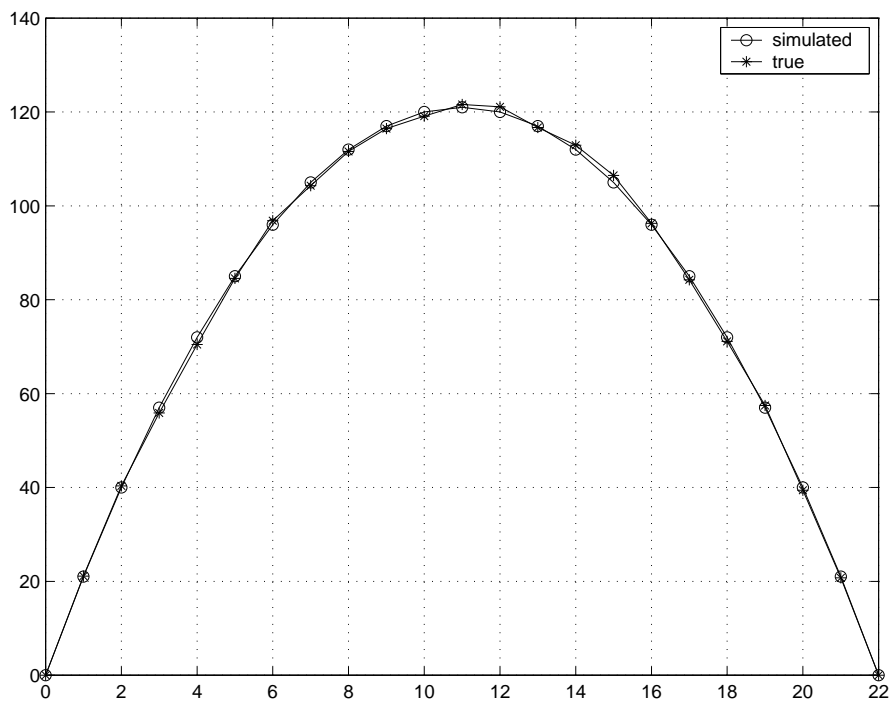


Figure 4.4: Histogram for the coalescence time for a silo of size 5

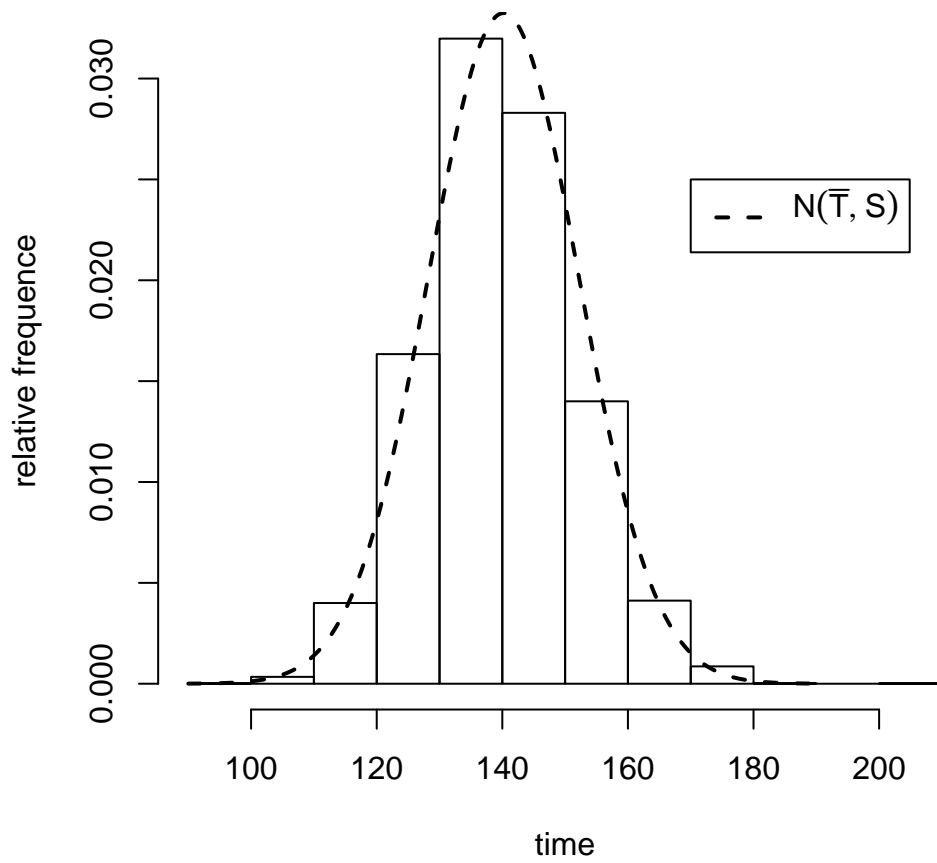


Figure 4.5: Histogram for the coalescence time for a silo of size 15

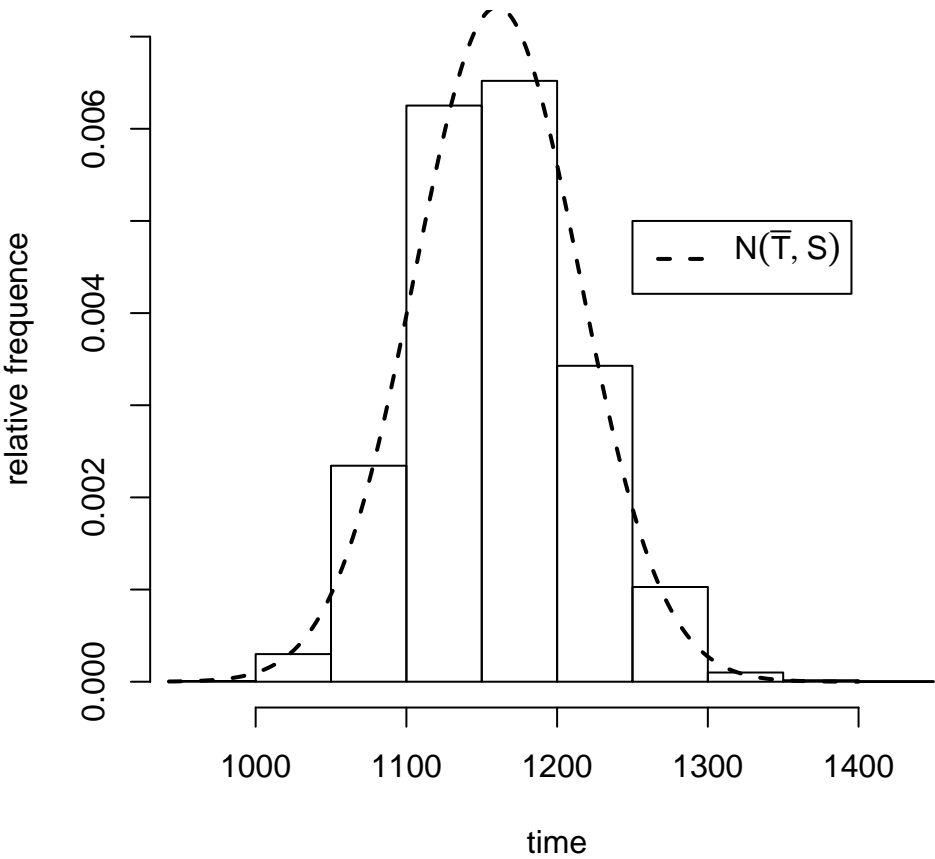


Figure 4.6: Histogram for the coalescence time for a silo of size 21

