Errors in Monte Carlo simulations using shift register random number generators

F. Schmid and N.B. Wilding

Institute für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany.

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Abstract

We report large systematic errors in Monte Carlo simulations of the tricritical Blume-Capel model using single spin Metropolis updating. The error, manifest as a 20% asymmetry in the magnetisation distribution, is traced to the interplay between strong triplet correlations in the shift register random number generator and the large tricritical clusters. The effect of these correlations is visible only when the system volume is a multiple of the random number generator lag parameter. No such effects are observed in related models.
I. INTRODUCTION

Interest in random number generator (RNG) deficiencies has recently been aroused by the work of Ferrenberg et al. [1], who found that the widely employed “R250” generator produces systematic errors in Monte Carlo simulations using cluster updating algorithms. Their high precision measurements of the specific heat and the internal energy of the critical two dimensional Ising model differed from the exact values by up to 0.05% [1].

These observations prompted a number of detailed studies of systematic errors in cluster algorithms and other “depth first” algorithms, such as those employed for simulating self avoiding walks [2]-[6]. The consensus emerging from these studies was that pseudo random numbers (PRNs) \( \{X_n\} \) generated by generalized feedback shift register (GFSR) algorithms of the type [7]

\[
X_n = X_{n-p} \oplus X_{n-q} \quad (\oplus \equiv \text{exclusive-or}),
\]

are generally “bad” when used in depth first algorithms, even though they pass many of the standard RNG tests and have very long periods [5]. However for local (single spin flip) Metropolis updating, good results were obtained using the GFSR generators. It was therefore concluded that this type of algorithm is relatively insensitive to correlations and thus safe to use.

In this paper, we show that in certain circumstances large systematic errors can also arise when using GFSRs generators in conjunction with local Metropolis updating. We demonstrate this for the case of the tricritical Blume-Capel model and argue that the observed errors originate from certain extremely large triplet correlations in the random number sequences.

II. RESULTS

There have been a number of recent suggestions in the literature that the problems observed with the GFSR generators may originate from triplet correlations [2,6]. In view
of this we have made a study of three point correlations in the GFSR generators and have
indeed found an extremely large effect in the \((X_n, X_{n-p}, X_{n-q})\) triplet. For this triplet the
three point average \(\langle X_n \cdot X_{n-p} \cdot X_{n-q} \rangle\) takes the value 0.107 instead of \((1/2)^3 = 0.125\). This
effect is displayed in figure 1 where we plot the triplets \(\langle X_n X_{n-k} X_{n-250} \rangle\) as a function of \(k\),
for \(1 \leq k \leq 249\). The results were obtained from a sequence of \(10^8\) PRNs using the magic
number pair \((250, 147)\) corresponding to the R250 generator. In fact the same effect, with
the same magnitude, is observable for other magic number pairs \((p, q)\) recommended in the
literature [7], viz \((521, 168), (1279, 216), (1279, 418), (3217, 67), (3217, 576), (4423, 1393),
(4423, 2098), (9689, 84), (9689, 471), (9689, 1836), (9689, 2444), (9689, 4187)\).

It is thus conceivable that triplet correlations are responsible for the systematic errors
observed in “depth first” algorithms, which principally rely on long uncorrelated sequences of
random numbers. However, as mentioned above, it has hitherto been generally believed that
local Metropolis updating schemes are insensitive to correlations in the PRN sequences and
give results at least better than linear congruential RNGs [1, 5]. In fact we have found that
in one system, the tricritical Blume-Capel model, triplet correlations can lead to extremely
large \((\sim 20\%)\) errors, even when using a Metropolis single site updating scheme.

The Blume-Capel model is a spin 1 Ising model with the Hamiltonian

\[
\mathcal{H}_{BC} = -\sum_{<ij>} s_i s_j + \Delta \sum_i s_i^2, \tag{2}
\]

where spins \(s_i\) take the values \(s_i = 0, \pm 1\) and the sum \(<ij>\) runs over all nearest neighbor
pairs. We have simulated this model on an FCC lattice for system size \(V = (5 \times 5 \times 5 \cdot 4) = 500\) spins. Spins were updated serially, each update requiring two random numbers:
one to choose the new spin, and one for the Metropolis step. The random numbers were
generated by the R250 RNG, having the magic number pair \((p=250, q=147)\). Figure 2(a)
shows the measured probability distribution of the magnetisation \(M = \sum_i s_i\) at the near-
tricritical parameters \(k_B T = 3.0, \Delta = 5.67\) (circles). Notwithstanding the symmetry of
the Hamiltonian under inversion of all spins \((\{s_i\} \rightarrow \{-s_i\})\), the distribution is clearly
asymmetric with respect to the “plus” and “minus” phases. We find, however, that if spins
are updated randomly instead of serially, the distribution becomes symmetric [figure 2(b)].

We believe that the observed asymmetry in $P(M)$ is related to the fact that for system size $V = 500$, the larger generator lag $p = 250$ is a factor of the system volume, so that a given spin is always updated with a random number having the same relative position within successive sequences of 250 PRNs. This view is supported by the following evidence:

- We find that the asymmetry in $P(M)$ disappears when other system sizes are simulated, e.g. $(14 \times 14 \times 14 \cdot 4) = 1372$.
- The asymmetry disappears for the $V = 500$ system size when one additional PRN is drawn and discarded after each Monte Carlo step (i.e. after a whole sweep through the lattice).
- The asymmetry disappears for the $V = 500$ system size when the R250 generator is substituted by the “R1279”, a GFSR RNG with the magic number pair (1279,216).
- The asymmetry reappears with the R1279, for the $V = 500$ system size when 279 additional PRNs are drawn and discarded after each Monte Carlo step.

We further believe that the asymmetry in $P(M)$ is a manifestation of the aforementioned triplet correlations in the PRN sequence $(X_n, X_{n-p}, X_{n-q})$. To substantiate this we performed a simulation using the lagged Fibonacci RNG \[ X_n = X_{n-p} + X_{n-q} \mod 2^{31} \quad \text{with} \quad (p, q) = (1279, 216), \quad (3) \]

which is formally similar to the “R1279”, but does not display the triplet correlation. Even after discarding 279 PRNs after each cycle, $P(M)$ remains symmetric with this generator.

It is interesting to observe that a number of further factors influence the size of the asymmetry effect. One is the proximity to the tricritical point. If we choose $\Delta = 0, k_B T = 6.8$, corresponding to the critical point of the spin 1 Ising model, the effect weakens, but remains clearly discernible (not shown). We also note that the asymmetry effect is not
influenced by the dimensionality or the type of lattice: Simulations of the $L = 10 \times 10$ Blume-Capel model on a square lattice (with 50 additional random numbers discarded between each sweep) exhibit the asymmetry with a similar magnitude to that observed in the three-dimensional case.

The effect does, however, seem to depend on the symmetry of the Hamiltonian of the model studied. To demonstrate this we have also performed simulations on the three state Potts model near its critical point. This is a lattice spin model with the Hamiltonian

$$\mathcal{H}_P = - \sum_{<ij>} \delta_{s_i,s_j},$$

where $\delta_{ij}$ denotes the Kronecker symbol and $s_i$ takes again the values $s_i = 0, \pm 1$. The sole alteration required to the Blume-Capel program to simulate this model, is the calculation of the energy change in the Metropolis step. In figure 3 we show the magnetisation distribution $P(M)$ for the three state Potts model on a $V = 500$ FCC lattice, for the near-critical temperature $k_B T = 3.9$. No asymmetry between the “plus” and “minus” phases is evident. Similar simulations on the 2D simple Ising model also reveal no asymmetry.

It is thus clear that the observed asymmetry in the tricritical Blume-Capel model is the result of a subtle interplay between the tricritical clusters and PRN triplet correlations. The fact that one of the three phases in the Blume-Capel model (the “0” phase) is distinguishable from the other two at the tricritical point seems to be crucial. From the joint distribution $p(M, Q)$, with $Q = \sum_i s_i^2$ (figure 4), one sees that there is no direct phase space path between the “plus” and “minus” phases. In order to migrate from one of these phases to the another, the system must pass through the “0” phase. It seems that the tricritical clusters of “0”s are very sensitive to correlations in the PRNs, and that “resonant enhancement” of the triplet correlations occurs when the system size is a multiple of the larger generator lag. The critical clusters in the Potts model are much less susceptible to these specific correlations.
III. CONCLUSIONS

To summarize, we have demonstrated that the interplay between the physical properties of a system (principally the system size) and random number generator triplet correlations can lead to strong systematic errors in simulations even when simple Metropolis updating is used. Such “resonant enhancement” of PRN correlations can be very specific to a particular situation, as in our case of the tricritical Blume-Capel model, and not be observable at all in other, albeit very similar systems. Our observation therefore supports the view that a random number generator is only “good” in conjunction with the specific application for which it has been tested – every new application is also a new pseudo random number test, where known and unknown correlations may gain importance in an uncontrolled way.

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FIGURES

FIG. 1. The triplets $\langle X_n X_{n-k} X_{n-250} \rangle$ as a function of $1 \leq k \leq 249$, generated from a sequence of $10^8$ PRNs using the generator of equation 1 with $p = 250$, $q = 147$.

FIG. 2. (a) Magnetisation distribution of the Blume Capel model on the $V = 500$ site FCC lattice at $k_B T = 3, \Delta = 5.67$, obtained using serial updating with the R250 generator. (b) The same distribution obtained using random site updating.

FIG. 3. Magnetisation distribution of the three state Potts model on the $V = 500$ FCC lattice at $k_B T = 3.9$, obtained with PRNs generated by the R250 RNG.

FIG. 4. The joint distribution $P(M, Q)$ of the near-tricritical Blume-Capel model. Also shown on the grid base is a contour plot of the histogram surface.
FIG. 1. The triplets $\langle X_n X_{n-k} X_{n-250} \rangle$ as a function of $1 \leq k \leq 249$, generated from a sequence of $10^6$ PRNs using the generator of equation 1 with $p = 250$, $q = 147$. 
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