Comment on
“Antiferromagnetic Potts Models”

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October 15, 2018

Abstract

We show that the Wang-Swendsen-Kotecký algorithm for antiferromagnetic $q$-state Potts models is nonergodic at zero temperature for $q = 3$ on periodic $3m \times 3n$ lattices where $m, n$ are relatively prime. For $q \geq 4$ and/or other lattice sizes or boundary conditions, the ergodicity at zero temperature is an open question.
Wang, Swendsen and Kotecký (WSK) [1] have recently proposed an elegant Monte Carlo
algorithm for simulating the antiferromagnetic $q$-state Potts model on a finite graph $G$. It
goes as follows: Choose at random two distinct “colors” $\alpha, \beta \in \{1, \ldots, q\}$; freeze all the spins
taking values $\neq \alpha, \beta$, and allow the remaining spins to take value either $\alpha$ or $\beta$. The induced
model is then an antiferromagnetic Ising model, which can be updated by any legitimate
algorithm (for example, the Swendsen-Wang algorithm [2] or Wolff’s single-cluster variant
[3]).

At zero temperature the antiferromagnetic $q$-state Potts model reduces to the equal-
weight distribution on $q$-colorings of $G$, and the WSK algorithm becomes: independently for
each connected cluster of $\alpha - \beta$ spins, either leave that cluster as is or else flip it (interchanging
$\alpha$ and $\beta$).

WSK studied their algorithm numerically for (among other cases) the $q = 3$ model at
$T = 0$ on square lattices of linear size $L = 4, 8, 16, 32, 64$ with periodic boundary conditions.
They claimed that the autocorrelation time was $\tau_{WSK} \approx 7$ independent of $L$, while the au-
tocorrelation time of a single-spin-flip algorithm increased approximately as $\tau_{SSF} \approx 0.32L^2$.

If the (exponential) autocorrelation time of a Monte Carlo algorithm is finite, then in
particular that algorithm must be ergodic. However, WSK did not give any proof of the
ergodicity of their algorithm at $T = 0$. (The ergodicity at $T \neq 0$ is trivial.) Here we show
that in fact the algorithm is not ergodic at $T = 0$ for $q = 3$ on periodic lattices of size
$3m \times 3n$ where $m, n$ are relatively prime. For $q \geq 4$ and/or other lattice sizes or boundary
conditions, the ergodicity at $T = 0$ is an open question.

Consider the configurations shown in Figure 1 for a $3 \times 3$ periodic lattice. For any choice
of $\alpha, \beta$, the sites colored $\alpha - \beta$ form a single connected cluster, so the only possible moves in
the WSK algorithm are global permutations of the colors. On the other hand, configurations
(a) and (b) are not related by a global permutation, since in (a) the bands of constant color
run northeast-southwest while in (b) they run northwest-southeast. It follows that the WSK
algorithm is nonergodic.

Next consider the configurations of Figure 1 repeated periodically on a $3m \times 3n$ lattice. If
$m, n$ are relatively prime, then the sites colored $\alpha - \beta$ form a single connected band winding
around the lattice, and the argument goes through unchanged. If $m, n$ are not relatively
prime, then the sites colored $\alpha - \beta$ form several disjoint connected bands, and the ergodicity
is an open problem.

We remark that these configurations are completely frozen under any single-spin-update

\begin{center}
\begin{array}{ccc}
1 & 2 & 3 \\
2 & 3 & 1 \\
3 & 1 & 2 \\
\end{array}
\end{center}

(a)

\begin{center}
\begin{array}{ccc}
1 & 2 & 3 \\
3 & 1 & 2 \\
2 & 3 & 1 \\
\end{array}
\end{center}

(b)

Figure 1: Configurations of the zero-temperature antiferromagnetic 3-state Potts model on
a $3 \times 3$ lattice with periodic boundary conditions.
algorithm, because each spin is surrounded by neighbors of both colors. So any such algorithm is also nonergodic. The same holds for $q = 4$ on lattices $4m \times 4n$, and for $q = 5$ on lattices $5m \times 5n$. For $q \geq 6$, the single-spin-update algorithm is easily seen to be ergodic on any square lattice \[4\]; more generally, this holds on an arbitrary graph $G$ for $q \geq \max \deg G + 2$.

We also remark that the WSK algorithm for $q = 3$ is nonergodic on the planar graph of Fig. 10.4.

To see these nonergodicities numerically requires some care:

(a) One must study the model not only at $T = 0$, but also at temperatures $T$ approaching zero; then one will see the autocorrelation time growing without limit.

(b) One must measure an observable that distinguishes between the ergodic classes. For example, in the above situation one could use $|\tilde{\sigma}(k)|^2$ at momenta $k = (2\pi/3, \pm 2\pi/3)$. It is not clear which observables might be sensitive to any possible nonergodicities at other values of $q$ and $L$.

It is an open question whether there exist efficient algorithms for simulating the anti-ferromagnetic Potts model at zero temperature for $q = 3, 4, 5$ (more generally, for $q < \max \deg G + 2$). Jerrum \[4\] has pointed out that it is unlikely that such algorithms (with polynomially bounded autocorrelation time measured in CPU units) can exist for arbitrary graphs $G$ and fixed $q$: indeed, the existence of such an algorithm for $q = 5$ would permit one to ascertain with high probability the 3-colorability of an arbitrary degree-4 graph, which is impossible if $\mathsf{NP} \neq \mathsf{RP}$ \[6\].

We wish to thank Mark Jerrum and Greg Sorkin for helpful correspondence.

References

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[6] For the definitions of $\mathsf{NP}$ and $\mathsf{RP}$, see M.R. Garey and D.S. Johnson, \textit{Computers and Intractability} (Freeman, San Francisco, 1979) and D.J.A. Welsh, Discrete Appl. Math. \textbf{5}, 133 (1983).