Comment on "Antiferromagnetic Potts Models"

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 α or β. 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 the following: independently for each connected cluster of α-β spins, either leave that cluster as is or else flip it (interchanging α and β).

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 $\tau_{\mathrm{WSK}} \approx 7$ independent of L, while the autocorrelation time of a single-spin-flip algorithm increased approximately as $\tau_{\mathrm{SSF}} \approx 0.32L^2$.

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 Fig. 1 for a 3×3 periodic lattice. For any choice of α,β, the sites colored α-β 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 Fig. 1 repeated periodically on a $3m\times 3n$ lattice. If m,n are relatively prime, then the sites colored α-β 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 α-β 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 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 $q \geq \max\deg G+2$.

1	2	3	1	2	3
2	3	1	3	1	2
3	1	2	2	3	1
	(a)			(b)	

FIG. 1. Configurations of the zero-temperature antiferromagnetic three-state Potts model on a 3×3 lattice with periodic boundary conditions.

We also remark that the WSK algorithm for $q=3$ is nonergodic on the *planar* graph of Ref. [5], 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. Thus, 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 antiferromagnetic 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 $NP\neq RP$ [6].

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