Rigorous Lower Bound on the Dynamic Critical Exponents of the Swendsen-Wang Algorithm

Xiao-Jian Li[(a)] and Alan D. Sokal[(b)]

Department of Physics, New York University, 4 Washington Place, New York, New York 10003

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We prove the rigorous lower bound $z_{SW} \geq \alpha/\nu$ for the dynamic critical exponent of the Swendsen-Wang algorithm. For two-dimensional q-state Potts models with $q=2,3,4$, this implies $z_{SW} \geq 0, \frac{2}{5}, 1$. We present numerical data indicating that $z_{SW} = 0.55 \pm 0.03$, 0.89 ± 0.05 for $q=3,4$ (95% confidence limits, statistical errors only). The discrepancy for $q=4$ appears to be caused by multiplicative logarithmic corrections.

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Monte Carlo computations of critical phenomena and quantum field theory have been greatly hampered by *critical slowing down*: The autocorrelation time τ of the traditional Monte Carlo algorithms—that is, roughly speaking, the time needed to produce one "statistically independent" field configuration—grows rapidly as the critical point is approached. In recent years much effort has gone into developing new Monte Carlo algorithms with radically reduced critical slowing down.[1]

Two years ago, Swendsen and Wang (SW)[2] proposed a Monte Carlo algorithm for Potts spin models that has extraordinarily small critical slowing down. But very little is understood at present, even heuristically, about the SW dynamics: One would like to know why the critical slowing down is so small, and why it is not eliminated entirely.

In this Letter we prove a rigorous lower bound for the autocorrelation time of the SW algorithm,

$$\tau \geq \text{const} \times C_H ,$$

where C_H is the specific heat. This implies the bound

$$z_{SW} \geq \alpha/\nu$$

for the dynamic critical exponent. It follows that critical slowing down cannot be entirely absent (if the specific heat diverges at criticality), and that in some cases (e.g., the four-state Potts model in two dimensions) it must be moderately severe. The physical mechanism underlying our proof is the slow equilibration of the bond density $\mathcal{N}$ and other "energylike" observables.

Let us first recall[3] that the SW algorithm simulates a joint model having Potts spins $\sigma_i = 1,2,\ldots,q$ at the sites and occupation variables $n_{ij}=0,1$ on the bonds, with Boltzmann weight

$$W_{\text{joint}}(\{\sigma\},\{n\}) = Z^{-1} \prod_{\langle ij \rangle} [(1-p_{ij})\delta_{n_{ij},0} + p_{ij}\delta_{n_{ij},1}\delta_{\sigma_i,\sigma_j}] , \tag{1}$$

where $0 \leq p_{ij} \leq 1$. It is trivial to verify that the marginal distribution of (1) on the Potts variables $\{\sigma\}$ (integrating out the $\{n\}$) is the ferromagnetic Potts model,

$$W_{\text{Potts}}(\{\sigma\}) = Z^{-1} \prod_{\langle ij \rangle} [(1-p_{ij}) + p_{ij}\delta_{\sigma_i,\sigma_j}]$$
$$= Z^{-1} \exp\left(\sum_{\langle ij \rangle} J_{ij}(\delta_{\sigma_i,\sigma_j} - 1) \right) ,$$

where $p_{ij} = 1 - \exp(-J_{ij})$. It is also easy to verify that the marginal distribution of (1) on the bond variables $\{n\}$ (integrating out the $\{\sigma\}$) is the random-cluster model[4] with parameter q,

$$W_{\text{RC}}(\{n\}) = Z^{-1} \left(\prod_{\langle ij \rangle : n_{ij}=1} p_{ij} \right) \left(\prod_{\langle ij \rangle : n_{ij}=0} (1-p_{ij}) \right) q^{\mathcal{C}(\{n\})} ,$$

where $\mathcal{C}(\{n\})$ is the number of connected components (including one-site components) in the graph whose edges are the bonds having $n_{ij}=1$. Moreover, the conditional distribution of the $\{n\}$ given the $\{\sigma\}$ is as follows: Independently for each bond $\langle ij \rangle$, one sets $n_{ij}=0$ in the case $\sigma_i \neq \sigma_j$, and sets $n_{ij}=0$ and 1 with probabilities $1-p_{ij}$ and p_{ij} in the case $\sigma_i = \sigma_j$. Finally, the conditional distribution of the $\{\sigma\}$ given the $\{n\}$ is as follows: Independently for each connected cluster, one sets all the spins σ_i in that cluster equal to the same value, chosen equiprobably from the set $\{1,2,\ldots,q\}$.

The SW algorithm simulates the joint model (1) by alternately applying the two conditional distributions—that is, by alternately generating new bond occupation variables (independent of the old ones) given the spins, and new spin variables (independent of the old ones) given the bonds. The transition matrix $P_{SW} = P_{SW} \times (\{\sigma,n\} \to \{\sigma',n'\})$ is therefore a product

$$P_{SW} = P_{\text{bond}} P_{\text{spin}} ,$$

where P_{bond} is the conditional expectation operator[5] $E(\cdot \mid \{\sigma\})$, and P_{spin} is $E(\cdot \mid \{n\})$.

Our strategy[6] will be to prove a lower bound on the autocorrelation time τ by computing explicitly the autocorrelation function at time lags 0 and 1 for a suitably chosen trial observable f, and then using general facts about reversible Markov chains. To obtain a good bound, it is necessary to choose an observable f that has

sufficiently strong overlap with the slowest model(s). We shall choose f to be the bond density

$$\mathcal{N} = \sum_{\langle ij \rangle} n_{ij} .$$

To lighten the notation, let us write $\delta_{\sigma_b} \equiv \delta_{\sigma_i,\sigma_j}$ for a bond $b = \langle ij \rangle$. We then have

$$E(n_b \mid \{\sigma\}) = p_b \delta_{\sigma_b} , \tag{2}$$

$$E(n_b n_{b'} \mid \{\sigma\}) = p_b p_{b'} \delta_{\sigma_b} \delta_{\sigma_{b'}} \text{ for } b \neq b' . \tag{3}$$

It follows from (2) that

$$\begin{aligned} \langle n_b(t=0) n_{b'}(t=1) \rangle &= \langle n_b E(E(n_{b'} \mid \{\sigma\}) \mid \{n\}) \rangle \\ &= \langle n_b E(n_{b'} \mid \{\sigma\}) \rangle \\ &= \langle E(n_b) \mid \{\sigma\}) E(n_{b'} \mid \{\sigma\}) \rangle \\ &= p_b p_{b'} \langle \delta_{\sigma_b} \delta_{\sigma_{b'}} \rangle . \end{aligned}$$

The corresponding truncated (connected) correlation function is clearly

$$\langle n_b(t=0); n_{b'}(t=1) \rangle = p_b p_{b'} \langle \delta_{\sigma_b}; \delta_{\sigma_{b'}} \rangle , \tag{4}$$

where $\langle A;B \rangle \equiv \langle AB \rangle - \langle A \rangle \langle B \rangle$. We have thus expressed a dynamic correlation function of the SW algorithm in terms of a static correlation function of the Potts model.

Now let us compute the same quantity at time lag 0: By (3), for $b \neq b'$ we have

$$\langle n_b(t=0) n_{b'}(t=0) \rangle = p_b p_{b'} \langle \delta_{\sigma_b} \delta_{\sigma_{b'}} \rangle$$

and hence

$$\langle n_b(t=0); n_{b'}(t=0) \rangle = p_b p_{b'} \langle \delta_{\sigma_b}; \delta_{\sigma_{b'}} \rangle . \tag{5}$$

On the other hand, for $b = b'$ we clearly have

$$\begin{aligned} \langle n_b(t=0); n_{b'}(t=0) \rangle &= \langle n_b \rangle - \langle n_b \rangle^2 \\ &= p_b \langle \delta_{\sigma_b} \rangle - p_b^2 \langle \delta_{\sigma_b} \rangle^2 . \end{aligned} \tag{6}$$

Consider now the usual case in which

$$p_b = \begin{cases} p & \text{for } b \in B, \\ 0 & \text{otherwise,} \end{cases}$$

for some family of bonds B. Combining (4)–(6) and summing over b, b', we obtain

$$\langle \mathcal{N}(t=0); \mathcal{N}(t=1) \rangle = p^2 \langle \mathcal{E}; \mathcal{E} \rangle ,$$

$$\langle \mathcal{N}(t=0); \mathcal{N}(t=0) \rangle = p^2 \langle \mathcal{E}; \mathcal{E} \rangle - p(1-p) \langle \mathcal{E} \rangle ,$$

where $\mathcal{E} \equiv -\sum_{b \in B} \delta_{\sigma_b} \leq 0$ is the energy. Hence the normalized autocorrelation function at time lag 1 is exactly

$$\rho_{\mathcal{N}\mathcal{N}}(1) \equiv \frac{\langle \mathcal{N}(t=0); \mathcal{N}(t=1) \rangle}{\langle \mathcal{N}(t=0); \mathcal{N}(t=0) \rangle} = 1 - \frac{-(1-p)E}{pC_H - (1-p)E} , \tag{7}$$

where $E \equiv V^{-1} \langle \mathcal{E} \rangle$ is the mean energy and $C_H \equiv V^{-1} \langle \mathcal{E}; \mathcal{E} \rangle$ is the specific heat (V is the volume). At criticality, $p \to p_{\text{crit}} > 0$ and $E \to E_{\text{crit}} < 0$, so

$$\rho_{\mathcal{N}\mathcal{N}}(1) \geq 1 - \text{const}/C_H . \tag{8}$$

This is the key inequality.

We now use general facts about reversible Markov chains, based on studying P_{SW} as an operator on the Hilbert space $L^2(W_{\text{joint}})$ defined by the inner product $(A,B) \equiv \langle AB \rangle$. Note first that

$$(\mathcal{N}, (P_{\text{bond}} P_{\text{spin}})^t \mathcal{N}) = (\mathcal{N}, (P_{\text{spin}} P_{\text{bond}} P_{\text{spin}})^t \mathcal{N})$$

for each $t \geq 0$, since $P_{\text{spin}}^2 = P_{\text{spin}}$ and $P_{\text{spin}}^* \mathcal{N} = P_{\text{spin}} \mathcal{N} = \mathcal{N}$. Thus, the correlation functions of $\mathcal{N}$ under P_{SW} are the same as those under $P'_{\text{SW}} \equiv P_{\text{spin}} P_{\text{bond}} P_{\text{spin}}$. This latter operator is a positive-semidefinite (in particular self-adjoint) contraction on $L^2(W_{\text{joint}})$, so we have a spectral representation

$$\rho_{\mathcal{N}\mathcal{N}}(t) = \int_0^1 \lambda^{|t|} \, d\nu(\lambda)$$

with a *positive* measure $d\nu(\lambda)$. It follows that

$$\rho_{\mathcal{N}\mathcal{N}}(t) \geq \rho_{\mathcal{N}\mathcal{N}}(1)^{|t|} .$$

Defining now the integrated autocorrelation time[1]

$$\tau_{\text{int},\mathcal{N}} \equiv \tfrac{1}{2} \sum_{t=-\infty}^{\infty} \rho_{\mathcal{N}\mathcal{N}}(t)$$

and the exponential autocorrelation time

$$\tau_{\text{exp},\mathcal{N}} = \lim_{|t| \to \infty} \frac{-|t|}{\ln \rho_{\mathcal{N}\mathcal{N}}(t)} ,$$

we conclude that

$$\tau_{\text{int},\mathcal{N}} \geq \frac{1}{2} \frac{1+\rho_{\mathcal{N}\mathcal{N}}(1)}{1-\rho_{\mathcal{N}\mathcal{N}}(1)} \geq \text{const} \times C_H \tag{9}$$

and

$$\tau_{\text{exp},\mathcal{N}} \geq \frac{-1}{\ln \rho_{\mathcal{N}\mathcal{N}}(1)} \geq \text{const} \times C_H . \tag{10}$$

In terms of the critical exponents defined by $\tau_{\text{int},\mathcal{N}} \sim \xi^{z_{\text{int}}}$, $\tau_{\text{exp},\mathcal{N}} \sim \xi^{z_{\text{exp}}}$, and $C_H \sim \xi^{\alpha/\nu}$ [or $L^{z_{\text{int}}}$, $L^{z_{\text{exp}}}$, and $L^{\alpha/\nu}$ for a system of linear size $L < \infty$ at criticality], we have

$$z_{\text{int}}, z_{\text{exp}} \geq \alpha/\nu . \tag{11}$$

For a first-order transition, Eqs. (9) and (10) imply that $\tau \geq \text{const} \times L^d$; the expected behavior is $\tau \sim \exp(cL^{d-1})$.

These same bounds hold for the autocorrelation function of the energy $\mathcal{E}$. In fact, we have the identity

$$(\mathcal{E}, (P_{\text{bond}} P_{\text{spin}})^t \mathcal{E}) = p^{-2} (\mathcal{N}, (P_{\text{spin}} P_{\text{bond}} P_{\text{spin}})^{t+1} \mathcal{N}) \tag{12}$$

for each $t \geq 0$, since $-p\mathcal{E} = P_{\text{bond}} \mathcal{N} = P_{\text{bond}} P_{\text{spin}} \mathcal{N}$. It follows easily that

$$\rho_{\mathcal{E}\mathcal{E}}(t) = \frac{\rho_{\mathcal{N}\mathcal{N}}(t+1)}{\rho_{\mathcal{N}\mathcal{N}}(1)} \geq \rho_{\mathcal{N}\mathcal{N}}(t) . \tag{13}$$

TABLE I. Comparison of z_{SW} with the rigorous lower bound α/ν. Estimates of z_{SW} are taken from Table II of this paper ($d=2$, $q=3,4$), Ref. 2 ($d=2,3$, $q=2$), and Ref. 7 ($d=4$, $q=2$). Error bars on z_{SW} are 95% confidence intervals. Values of α/ν are taken from Refs. 8 and 9.

	$d=2$ $q=2$	$d=2$ $q=3$	$d=2$ $q=4$	$d=3$ $q=2$	$d=4$ $q=2$
z_{SW}	≈ 0.35	0.55 ± 0.03	0.89 ± 0.05(!)	≈ 0.75	≈ 1
α/ν	$0\times\log$	$\frac{2}{5}$	$1\times\log^{-3/2}$	0.165 ± 0.02	$0\times\log^{1/3}$

Relations analogous to Eqs. (12) and (13) hold in fact for any observable $A(\{n\})$ and the corresponding improved estimator $\tilde{A} \equiv P_{\text{bond}}A = P_{\text{bond}}P_{\text{spin}}A$ [or $A(\{\sigma\})$ and $\tilde{A} \equiv P_{\text{spin}}A = P_{\text{spin}}P_{\text{bond}}A$]. They show that the normalized autocorrelation function (hence the autocorrelation time) of $\tilde{A}$ is larger than or equal to that of A, while the unrenormalized autocorrelation function (hence the error bar on the static mean) of $\tilde{A}$ is strictly smaller than that of A (but not much smaller if $\tau_{\text{int},A} \gg 1$.

In Table I we compare numerical estimates of z_{SW} with the known values (exact or approximate) of α/ν. The bound $z_{SW} \geq \alpha/\nu$ is clearly far from sharp for the Ising models ($q=2$); in particular, it fails to elucidate why (apparently) $z_{SW}=1$ for $d \geq 4$.[10] On the other hand, the bound is quite strong for the two-dimensional three- and four-state Potts models. Indeed, the bound *contradicts* the numerical estimate for the four-state Potts model (see below for discussion).

Our raw data for the two-dimensional Potts models are presented in Table II. All runs are 500000–1000000 sweeps; the first 5000 sweeps are discarded for equilibration. We verified the identity (7) to high precision. The integrated autocorrelation times $\tau_{\text{int},\mathcal{E}}$ and $\tau_{\text{int},\mathcal{N}}$ are estimated by standard procedures of statistical time-series analysis.[11] The exponent estimates z_{SW} are obtained by least-squares regression with a pure power law.

The anomalously low estimate of z_{SW} for $q=4$ is most likely caused by multiplicative logarithmic corrections. The specific heat C_H is known[8] to behave as $\sim L/\log^{3/2}L$, which could masquerade as a pure power $L^{\approx 0.7}$ for the range of L values considered here. Indeed, a power-law fit to our estimates of C_H yields the exponent $\alpha/\nu = 0.75(0.01)$. It appears that τ is rising slightly faster than C_H, but we are unable to distinguish between $z_{SW} > 1$ and $z_{SW} = 1$ with a smaller inverse power of logarithm. Accurate measurements on very large lattices could be useful. It is important for conceptual purposes to know whether the bound (11) is sharp for $q=4$.

The bound $\tau \geq \text{const} \times C_H$ can also be proven for the single-bond heat-bath algorithm[12] for the random-cluster model, at least with random (rather than sequential) bond updating. It would be interesting to know whether this algorithm belongs to the same dynamic universality class as the Swendsen-Wang algorithm.

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TABLE II. Integrated autocorrelation times for the SW algorithm on two-dimensional Potts models at the bulk critical temperature $J_{\text{crit}} = \ln(1+q^{1/2})$. All runs are 500000–1000000 sweeps; the first 5000 sweeps are discarded for equilibration. Standard error is shown in parentheses. Error estimates on z_{SW} include statistical error only.

	$q=3$	$q=4$	
L	$\tau_{\text{int},\mathcal{E}}$	$\tau_{\text{int},\mathcal{E}}$	$\tau_{\text{int},\mathcal{N}}$
16	9.0(0.2)	19.1(0.6)	17.7(0.5)
32	14.0(0.4)	36.7(1.6)	34.8(1.4)
64	19.3(0.6)	62.9(3.5)	60.8(3.3)
128	30.3(1.2)	115.7(6.1)	113.2(5.9)
256	39.6(1.7)	232.0(24.6)	229.2(24.2)
z_{SW}	0.55(0.02)	0.87(0.02)	0.90(0.02)

[a]Internet address: lixj @ act4.nyu.edu.

[b]Internet address: sokal @ act4. nyu.edu.

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