Binder Cumulants for the Ising Model using Worm algorithms

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The Worm Algorithm

In 2001, Prokof'ev and Svistunov proposed a *Worm Algorithm* for classical statistical models [1] that eliminates the problem of slowing at the critical point seen in traditional spin flip methods. Using high temperature expansions we move to a new configuration space of closed paths, whose evolution in time we simulate through the motion of the end points of a disconnected path. As an alternative to cluster or spin flip methods, the Worm algorithm is based on radically different principles and as such, has another range of potential applications. The closed path representation allows for the calculation of direct Monte Carlo estimators which are not available through the standard site representation. Taking such high-temperature expansions/duality transformations, we obtain the partition function for the enlarged ensemble:

$$\mathcal{Z}_1 = \sum_{\substack{u,v \\ \{k_l\}}} \frac{\Theta(k;u,v)}{\rho(u,v)} e^{-\mu \sum_l k_l}, \tag{1}$$

where the closed loop constraint $\Theta(k;u,v)$ is described by:

$$\Theta(k;u,v) = \prod_{y \notin \{u,v\}} \theta(k;y) \times \begin{cases} \theta(k;u) & \text{if} \quad u = v, \\ \bar{\theta}(k;u)\bar{\theta}(k;v) & \text{else.} \end{cases} \tag{2}$$

with

$$\theta(k;y) = \begin{cases} 1 & \text{if } \sum_{l,\partial l \ni y} k_l = \text{even}, \\ 0 & \text{else}, \end{cases} \tag{3}$$

and complement

$$\bar{\theta}(k;y) = 1 - \theta(k;y). \tag{4}$$

Update Scheme

- **Move:** Pick one of the v's nearest neighbours with equal probability and denote it v' with connecting link l. The proposed move is then $v \to v'$ with simultaneous adjustment $k_l \to 1 - k_l$ and is accepted with the Metropolis probability:

$$p_{\text{acc}} = \min\left(1, \frac{\rho(u,v)}{\rho(u,v')}\, e^{\mu(2k_l - 1)}\right), \tag{5}$$

  otherwise the original configuration is maintained. Since the update and system are translationally invariant, we only need to move v and can keep u fixed.

- **Kick:** If the system is in a configuration with $u = v$, we 'kick' the coincident pair to another randomly chosen lattice site with unchanged $\{k_l\}$ (no links are changed) with probability $0 < p_{\text{kick}} < 1$. For the dominant case where $u \neq v$, we do nothing in this step.

Fig. 1: Successful **Move** and **Kick** updates

Two Worm Extension

As an extension to the worm algorithm, we should be able to add a second "worm" to the system by adding two more lattice sites w, z to the set of points we keep track of with each update:

$$\{u, v\} \to \{u, v, w, z\}.$$

The natural extension of our partition function to a two worm system is then

$$\mathcal{Z}_2 = \sum_{\substack{u,v \\ w,z}} \sum_{\{\sigma\}} \sigma_u \sigma_v \sigma_w \sigma_z \frac{e^{-\beta E(\sigma)}}{\rho\,(u,v,w,z)}, \tag{6}$$

where we now keep track of four worm ends instead of two. Our update scheme then is largely the same as we keep the same **move** update from the original method. We will run without a **kick** update however as time constraints have prevented us from fully constructing and testing a consistent kick method that satisfies detailed balance. Thankfully, the lack of a kick update will only slightly increase our autocorrelation times, still giving a correct algorithm.

Binder Cumulants

A frequently used method to determine critical points of phase transitions in various physical systems is to use the intersection points of *Binder Cumulants* [2]. The most important advantage of the Binder Cumulant method is that finite size effects are much reduced. The 4th order Binder Cumulant U_L is defined as

$$U_L = 1 - \frac{\langle \bar{\sigma}^4 \rangle}{3\langle \bar{\sigma}^2 \rangle^2}, \tag{7}$$

where $\bar{\sigma}$ is the average spin given by $\bar{\sigma} = \frac{1}{L^2} \sum_i \sigma_i$ for the 2-dimensional square lattice Ising model.

Locating the critical point using U_L is then very easy. Using various lattice volumes, L^d, U_L's must be calculated as functions of β. Then, the intersection points where $U_L(\beta)$ curves cross will give the critical point β_c. Usually, it is helpful to find the crossings using ascending *pairs* of volumes $\left(\frac{L_1}{L_2}, \frac{L_2}{L_3}, \dots \text{ where } L_1 < L_2 < L_3 < \cdots\right)$ (fig. 5).

Numerical Results

Comparing the algorithms

Fig. 2 shows τ_{int} for two worm ends coinciding, $\langle \delta_{uv} \rangle_2$, at the critical temperature for lattices of size $L = 16$ & 256. Immediately, we see that autocorrelation times have improved for the two worm method over the single worm algorithm and as the lattice size, L, is increased, the improvement over what is an already very efficient algorithm increases. Looking at figs. 2 and 3, we see how the autocorrelation time for finding all four worm ends coinciding ($\tau_{\text{int,four}}$) converges to a minimum value of 0.5 for large L.

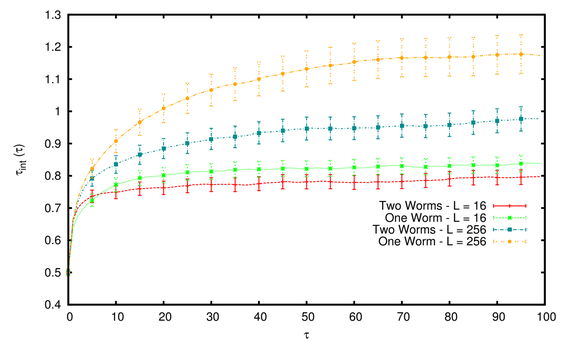

Fig. 2: Integrated autocorrelation for two worm ends coinciding at β_c for $L = 16, 256$ - One worm vs Two worm

In fig. 3 we have plotted the maximum/asymptotic value for τ_{int} as a function of L for both $\langle \delta_{uv} \rangle_2$ and $\langle \delta_{uv}\delta_{wz} \rangle_2$. At β_c, we see that $\tau_{\text{int,two}}$ scales at L^{ξ}, much like with the single worm method but with dynamical critical exponent $\xi_{\text{two}} = 0.000780 \pm 0.000055$, an order of magnitude closer to zero than for the single worm algorithm. Similarly for $\tau_{\text{int,four}}$ we have $\xi_{\text{four}} = -0.000332 \pm 0.000157$, closer again to zero scaling. Again, we see a complete absence of critical slowing down for primary observables.

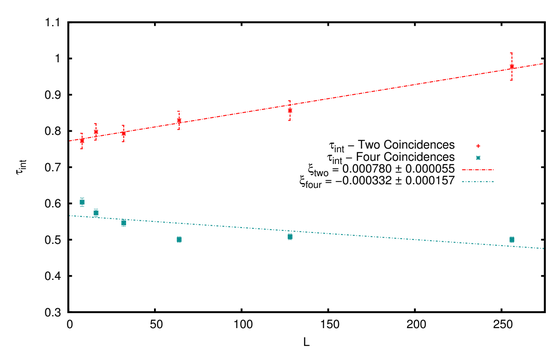

Fig. 3: Integrated autocorrelation times for $L = \{16, \dots, 256\}$ at β_c

Binder Cumulants

In fig. 4 we have plotted U_L against β for various lattice sizes which show, much like in our plots of χ, how as L increases, the slope of U_L increases and approaches a sharp peak at the critical temperature/phase transition point β_c. As expected, in the broken phase ($\beta > \beta_c$) U_L levels off around the theoretical value of $\frac{2}{3}$, behaving exactly how we expect. Intersection points of Binder Cumulants for ascending volume pairs are often used to determine the critical point, β_c, often giving more accurate results than the maximum locations of magnetic susceptibility as finite size effects are greatly reduced. In fig. 5 we look at the temperature at which these intersections occur and plot them against $1/L_{\text{min}}$ where L_{min} is the smaller lattice size of the coincident pair. The largest pair, $\frac{128}{256}$, gives a value for the critical temperature of $\beta = 0.440182(12)$, close to the known analytic value of $\beta_c = \frac{\ln(1+\sqrt{2})}{2} \approx 0.440686$.

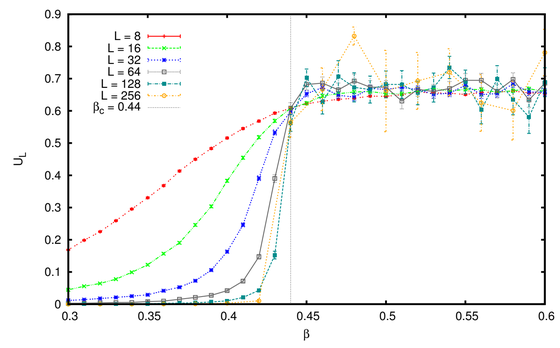

Fig. 4: Binder Cumulants against β for $L = \{16, \dots, 256\}$

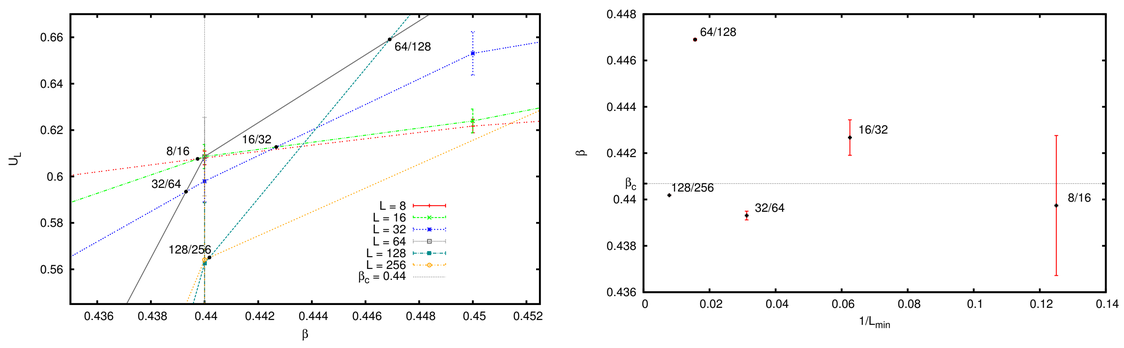

Fig. 5: Binder Cumulant intersections for $L = \{16, \dots, 256\}$

References

[1] N. Prokof'ev and B. Svistunov, "Worm Algorithms for Classical Statistical Models," *Physical Review Letters*, vol. 87, p. 160601, Oct. 2001.

[2] K. Binder, "Finite size scaling analysis of ising model block distribution functions," *Zeitschrift für Physik B Condensed Matter*, vol. 43, no. 2, pp. 119–140, 1981.