P 262 Pset 6

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1. Metropolis Simulation

a.

From the Metropolis Algorithm, we let C and C' be any two configurations that differ at one atom site. (assuming state C' is lower energy than state C, without loss of generality):

$$W(C \to C') = 1 \tag{1}$$

$$W(C' \to C) = e^{-\beta \delta E} \tag{2}$$

$$\delta E = E(C) - E(C') > 0 \tag{3}$$

Now, for a finite system we can transition from any state to any other state through a finite string of single-atom changes. Let us define a specific path W^*:

$$W^*(C \to C') = \Pi_{i=0}^{N-1} W^*(C_i \to C_{i+1}) \tag{4}$$

As a finite product of positive numbers, this probability is strictly greater than zero for any C and C', so Metropolis is ergodic! To check it satisfies detailed balance:

$$\frac{W^*(C \to C')}{W^*(C' \to C)} = \frac{\prod_{i=0}^{N-1} W^*(C_i \to C_{i+1})}{\prod_{i=N}^{0} W^*(C_i \to C_{i-1})} = \frac{\prod_{\delta E > 0} e^{-\beta \delta E}}{\prod_{\delta E' > 0} e^{-\beta \delta E'}} \tag{5}$$

Here δE and $\delta E'$ are ONLY the positive values in that "direction" from state C to C', as negative changes in energy contribute $W = 1$ and can be ignored in the product. But we note that $\delta E' = -\delta E$ at the same i step, thus:

$$\frac{W^*(C \to C')}{W^*(C' \to C)} = \frac{\prod_{\delta E > 0} e^{-\beta \delta E}}{\prod_{\delta E < 0} e^{\beta \delta E}} = \prod_{i=0}^{N-1} e^{-\beta \delta E} = e^{-\beta \sum_{i=0}^{N-1} \delta E} = e^{-\beta \Delta E} \tag{6}$$

$$W(C \to C') = \sum_{paths} W^*(C \to C') = \sum_{paths} W^*(C' \to C) e^{-\beta \Delta E} = \tag{7}$$

$$e^{-\beta \Delta E} \sum_{paths} W^*(C' \to C) = e^{-\beta \Delta E} W(C' \to C) \tag{8}$$

Which is the required detailed balance relationship.

b.

Figure 1: MCMC time evolution of Ising systems of varying sizes. Blue is above the critical temperature, green is at the critical temperature, and red is below the critical temperature.

Equilibrium appears to occur very rapidly in small systems, and on the order of 500 steps for larger ones. Equilibrium time of course depends on how close our system is to the critical temperature.

c.

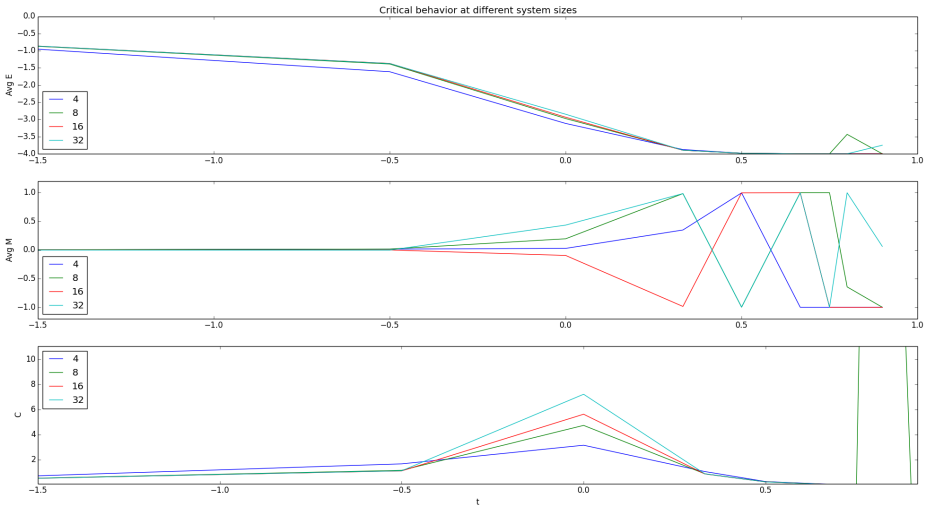

Figure 2: Critical behavior in Energy, Magnetization, and Heat Capacity for various system sizes. The Heat Capacity has the most pronounced behavior near criticality (t = 0) as it begins to show singular nature.

We expect the maximal heat capacity to be a constant with system size, but it appears to "increase" at t = 0. One interpretation is that the "exact" critical temperature from Onsager is not the critical temperature for finite systems. This would mean $T_c(n)$, where n is the system size, should decrease with n and converge to exact critical temperature as n approaches infinity. To investigate this we would need to sample many temperatures near T_c, but this represented too much computation time.

d.

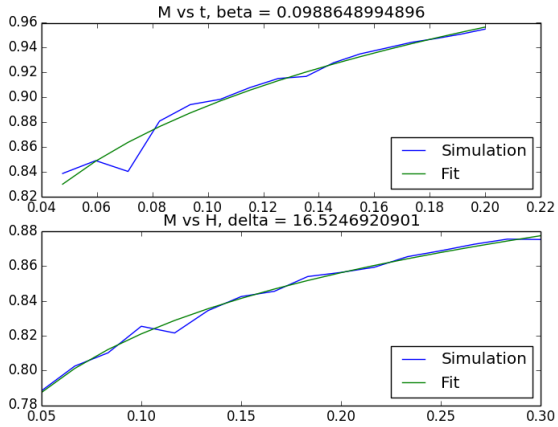

Figure 3: Simulation of Critical Exponents, $\beta = 0.099$ (exact $= 0.125$) and $\delta = 16.52$ (exact $= 16$)

e.

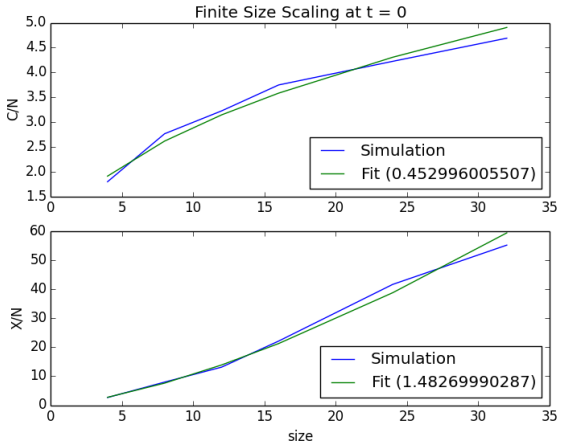

Figure 4: Finite Size Scaling methods to evaluate $\alpha/\nu = 0.45$ (exact $= 0$) and $\gamma/\nu = 1.48$ (exact $= 1.75$).

γ/ν agrees pretty well, but α/ν does not. Similar to the problem in part c), we are not sampling the actual maximal value for C/N, but rather the value for C/N at the exact critical temperature T_c. We would need to do a finer sweep over β to find a (hopefully) better estimate for both ratios.

2. Swendsen-Ma MCRG

Tabled values of ν for n=2 and n=3 normalization steps (starting from a 16x16 grid). We computed these using only nearest-neighbor (nn) coupling, and also with next-nearest-neighbor coupling (nnn). We performed an ensemble average over 25000 samples.

2 (nn only)	2 (nnn)	3 (nn only)	3 (nnn)
1.07083	0.98187	1.08363	0.69384

All but the n=3 (nnn) value match the exact result quite well ($\nu = 1$). This is most likely caused by the fact that the 3rd normalization step goes to a 2x2 system, and so the next-nearest-coupling causes a lot of self-coupling for each site. In the mean field case, $\nu = 1/2$, in the Migdall-Kadanoff construction, $\nu = 0.7472$, so we see that our simulation gives a much better estimate than these zeroth and first order approximation methods.

Code

Our code can be found in the repository: `https://github.com/stcarr/p262_metropolis`