Monte Carlo

Jin Liang

November 1, 2015

1 Simple sampling of the 2D-Ising model

1.1 Answer to the questions

1.1.1 Total magnetization M and nearest-neighbour coupling NNC

The maximal value for the total magnetization $M = \sum_i S_i$ is N, and the minimal value $-N$, when all the sites have spin up or spin down at the same time.

Because every site has four nearest neighbours, considering double counting, for the nearest-neighbour coupling $NNC = \sum_{<i,j>} S_i S_j$, the maximal value is $2N$, the minimal value is $-2N$.

1.1.2 Density of state

For simple sampling, the density of state $D(M, NNC) = \sum_i \delta_{M,M(S_i)} \delta_{NNC,NNC(S_i)}$. It is a histogram representing how often the system has reached the magnetization M and the nearest-neighbour coupling NNC.

1.1.3 Average

Thermodynamic average of a variable $X(M, NNC)$,

$$< X > (T) = \frac{\sum_{M,NNC} D(M,NNC) e^{-\beta H(M,NNC)} X(M,NNC)}{\sum_{M,NNC} D(M,NNC) e^{-\beta H(M,NNC)}}$$

Since $H = -J \sum_{<i,j>} S_i S_j$, in reduced units,

$$< X > (T) = \frac{\sum_{M,NNC} D(M,NNC) e^{NNC/T} X(M,NNC)}{\sum_{M,NNC} D(M,NNC) e^{NNC/T}}$$

It is better to evaluate the root-mean squared magnetization $\overline{M}(T) = \sqrt{< M^2 >}$, instead of the mean magnetization $< M >$ because M could be positive and negative. So when we sum up, different terms may cancel.

1.1.4 Probability

The size of the phase space, the total number of configurations, is 2^N. The probability to generate a configuration with $M = 0$ is,

$$P(M = 0) = \frac{C_N^{N/2}}{2^N}$$

with $M = M_{max}$ is,

$$P(M = M_{max}) = \frac{1}{2^N}$$

1.2 Results: $M(T)$ and D computed from different number of configurations

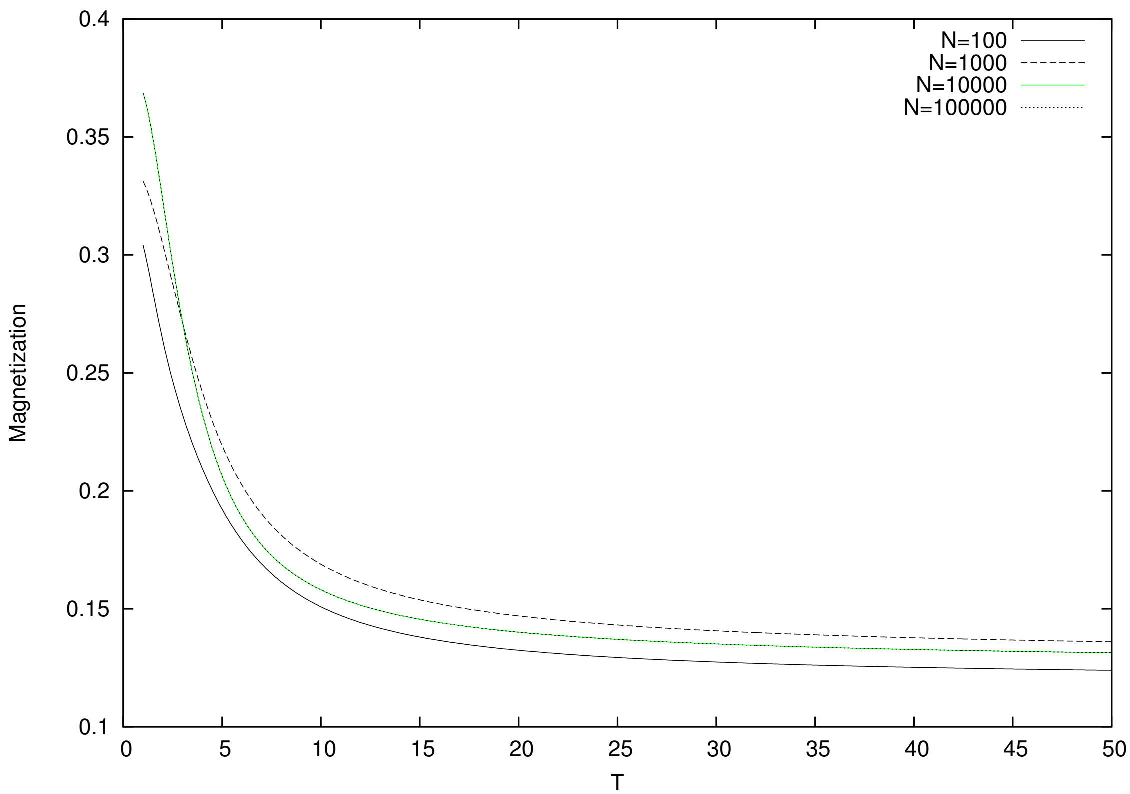

Figure 1: M_{rms} for different number of configurations

As the number of random configurations grows, the standard error decreases from the order of 10^{-3} to 10^{-4}. For a lattice of infinite size, M_{rms} should approximate to 0 at high temperature. For the 8×8 lattice, M_{rms} approximates to a finite value instead of 0. [Fig.1]

And as shown in Fig.2, The majority of the sampled configurations are in the centre of (M, NNC) space.

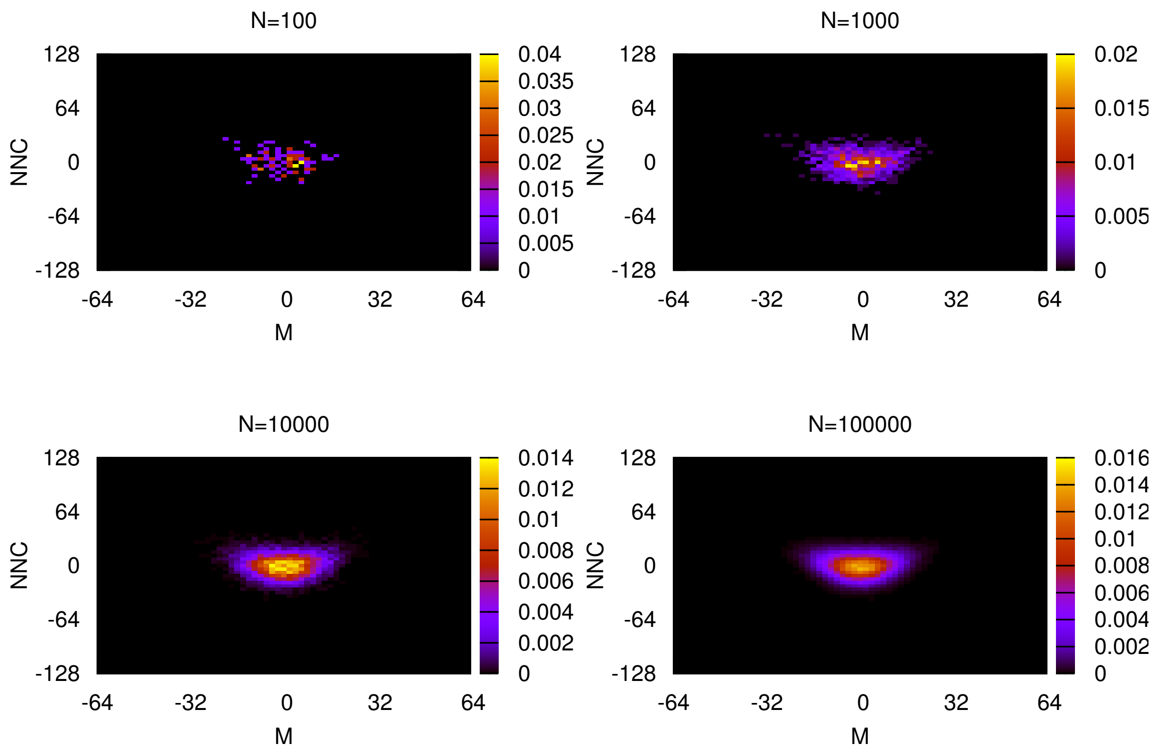

Figure 2: Density of state for different number of configurations

1.3 Solving 2D Ising model with simple sampling

The distribution of the configuration respect to M is a polynomial distribution, it is very unlikely for M to be far away from 0. When sampling all the possible configurations, there is a large degeneracy for configurations with $M \approx 0$.

2 Importance sampling

2.1 Introduction

2.1.1 Generate new configuration

In simple sampling, a large proportion of the sampling leads to configurations with M and NNC close to zero. Metropolis process makes it more likely to sample configurations with larger NNC.

First, we generate a random matrix.

Next, we randomly choose a site and flip the spin, and calculate the energy difference of the new configuration and the old one,

$$dE = H_n - H_o = (-NNC_n) - (-NNC_o)$$

Then, we use the metropolis scheme as the acceptance rule,

$$acc(o \to n) = min\{1, e^{-dE/T_0}\} = min\{1, e^{NNC_n - NNC_o/T_0}\}$$

There is a higher acceptance rate when NNC becomes larger.

2.1.2 Build the histogram $N_0(M, NNC)$

In simple sampling, we generate random configurations each time, but in importance sampling, we flip the spin to generate different configurations. Each time when we propose to flip the spin, that is, after each metropolis process, we update the histogram, wether or not the proposal is accepted.

Thermodynamic average of variable $X(M, NNC)$,

$$< X > (T_0) = \frac{\sum_{M,NNC} N_0(M,NNC)X(M,NNC)}{\sum_{M,NNC} N0(M,NNC)}$$

Standard deviation of the estimation

$$\delta_X = \sqrt{\frac{1}{N-1}(< X^2 > - < X >^2)} = \sqrt{\frac{1}{N-1}[\frac{\sum_i {X_i}^2}{N} - (\frac{\sum_i X_i}{N})^2]}$$

For the standard deviation of M, we first calculate the standard deviation of M^2,

$$\delta_{M^2} = \sqrt{\frac{1}{N_{flip}-1}(< M^4 > - < M^2 >^2)}$$

then we calculate the standard deviation of $\sqrt{M^2}$ with error propagation,

$$\delta_{\sqrt{M^2}} = \frac{\partial\sqrt{<M^2>}}{\partial <M^2>}\delta_{M^2} = \frac{1}{2\sqrt{<M^2>}}\delta_{M^2}$$

2.1.3 Density of State $D(M, NNC)$

If we want to get the thermodynamic average at temperature T_1 from data collected at T_0, we use data reweighting.

The density of state is

$$D(M, NNC) = N_0(M, NNC)e^{\frac{H}{kT_0}}$$

The thermodynamic average at temperature T_1 is

$$\begin{aligned} < M^2 >_1 &= \frac{\sum_i {M_i}^2 e^{-\beta_1 H_i}}{\sum_i e^{-\beta_1 H_i}} \\ &= \frac{\sum_i {M_i}^2 e^{-(\beta_1-\beta_0)H_i} e^{-\beta_0 H_i}}{\sum_i e^{-(\beta_1-\beta_0)H_i} e^{-\beta_0 H_i}} \\ &= \frac{\sum_{M,NNC} M^2 e^{-\beta_1 H} e^{\beta_0 H} N_0(M,NNC)}{\sum_{M,NNC} e^{-\beta_1 H} e^{\beta_0 H} N_0(M,NNC)} \\ &= \frac{\sum_{M,NNC} M^2 e^{-\beta_1 H} D(M,NNC)}{\sum_{M,NNC} e^{-\beta_1 H} D(M,NNC)} \end{aligned}$$

When calculating the standard error of M_{rms}, we need to take data reweighting into consideration. Suppose ω_ν is the Boltzman weight at the expected temperature, p_ν the probability to generate the configuration, the standard error is calculated as,

$$\delta^2 = \text{Variance}\frac{\sum_\nu (\frac{\omega_\nu}{p_\nu})^2}{(\sum_\nu \frac{\omega_\nu}{p_\nu})^2}$$

In our specific case,

$$\delta^2(M^2) = \text{Variance}(M^2)\frac{\sum_{M,NNC}(\frac{e^{-\beta H}}{e^{-\beta_0 H}})^2 N_0(M,NNC)}{(\sum_{M,NNC}\frac{e^{-\beta H}}{e^{-\beta_0 H}} N_0(M,NNC))^2}$$

$$\delta_{\sqrt{M^2}} = \frac{1}{2\sqrt{<M^2>}}\delta_{M^2}$$

$$\text{Variance}(M^2) = \sqrt{< M^4 > - < M^2 >^2}$$

2.2 Results

2.2.1 $M(T_0)$, $N_0(M, NNC)$ for different T_0

As shown in Fig.3, $M(T_0)$ calculated from different T_0 decreases. This is consistent with M_{rms} calculated from data reweighting. [Fig.5]

The histograms $N(M, NNC)$ for different T_0 is shown in Fig.4, the configurations are biased to large NNC area, that is, to low energy. This bias is stronger for low T_0. This is because according to the acceptance rule,

$$acc(o \to n) = min\{1, e^{-dE/T_0}\} = min\{1, e^{NNC_n - NNC_o/T_0}\}$$

when T_0 is small, it goes to larger NNC very fast, and it is very unlikely to go backwards to small NNC. But for large T_0, there is not a large discrepancy.

This can also be seen in the histogram of M [Fig.5], for $T_0 = 1.5$ and $T_0 = 2$, the majority of the sampling goes to large $|M_{rms}|$. And when it goes to one end of M, it is trapped, very difficult to go backwards. This can also be used to indicate the critical temperature. Below T_c, the two domains of $+M$ and $-M$ are isolated, but above T_c, they are connected.

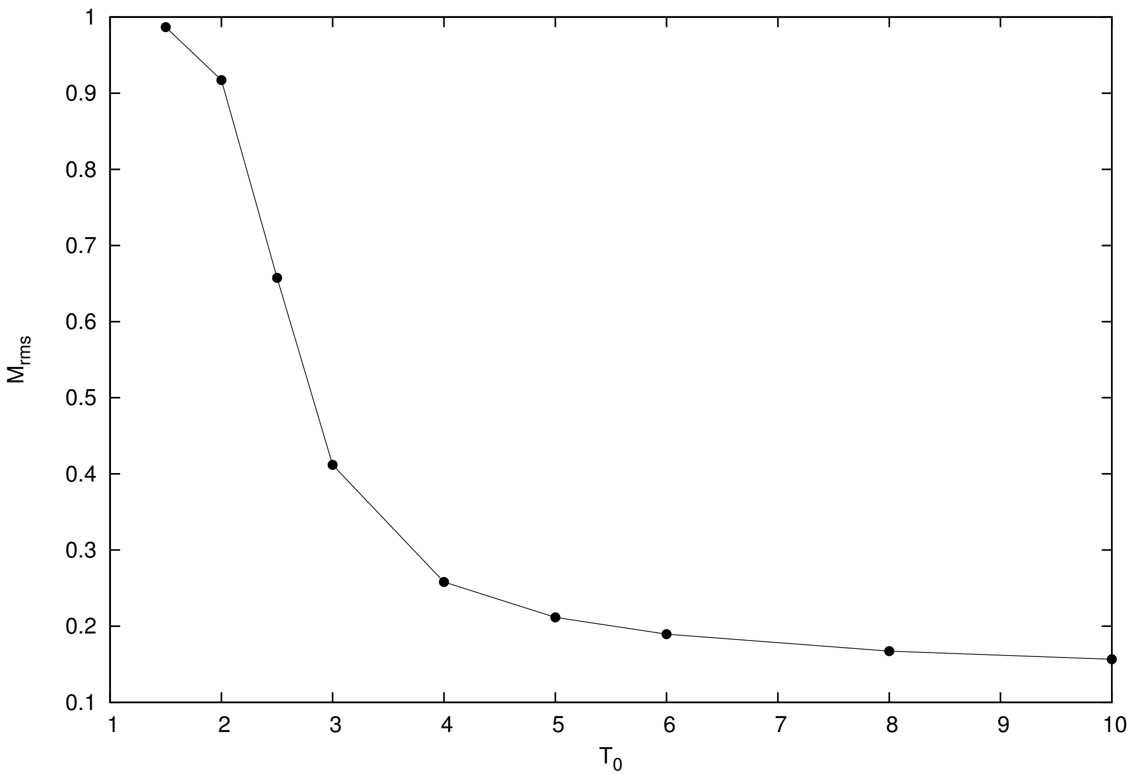

Figure 3: $M(T_0)$ for different T_0

2.2.2 Evolution of $M(T)$ for different T_0

The evolution of $M(T)$ for different T_0 is collected in Fig.6. When close to T_c, there is a deep drop of $M(T)$.

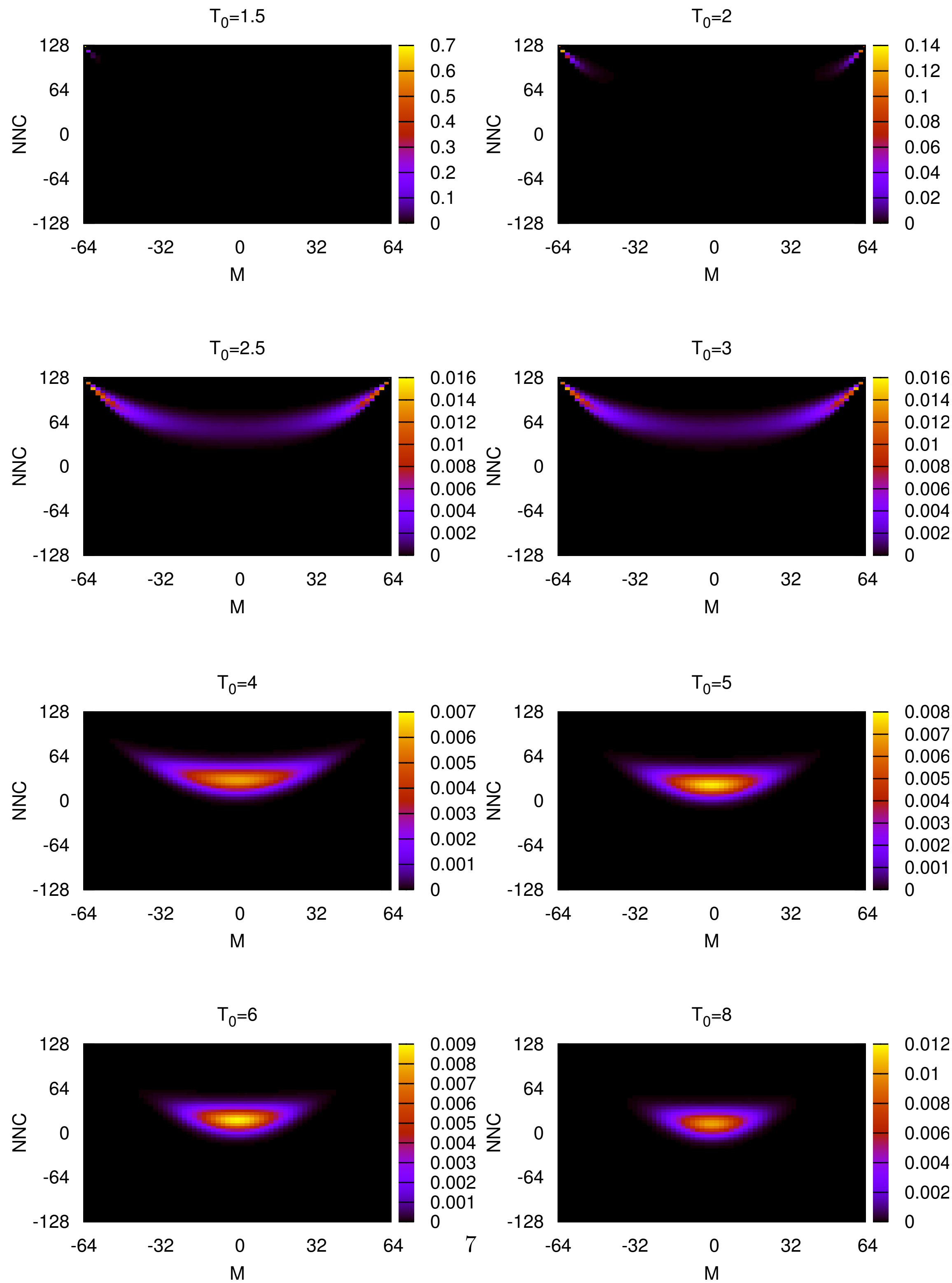

Figure 4: Histogram $N(M, NNC)$ for different T_0

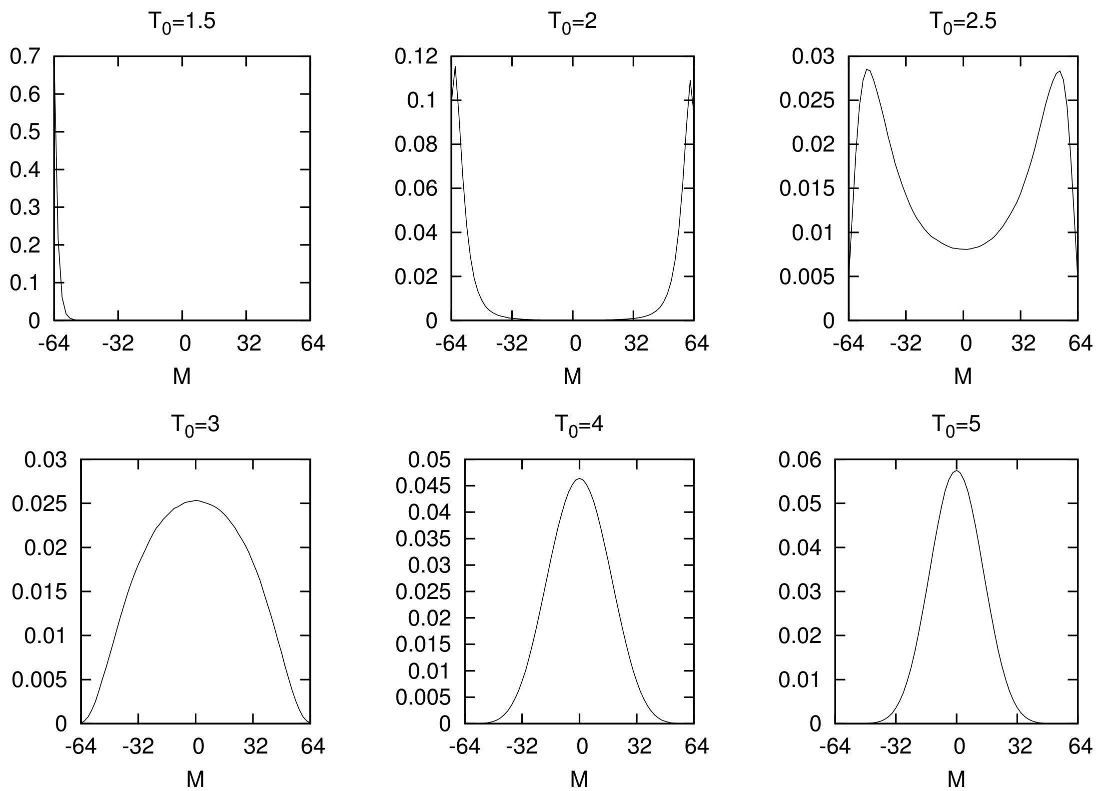

Figure 5: Histogram of M for different T_0

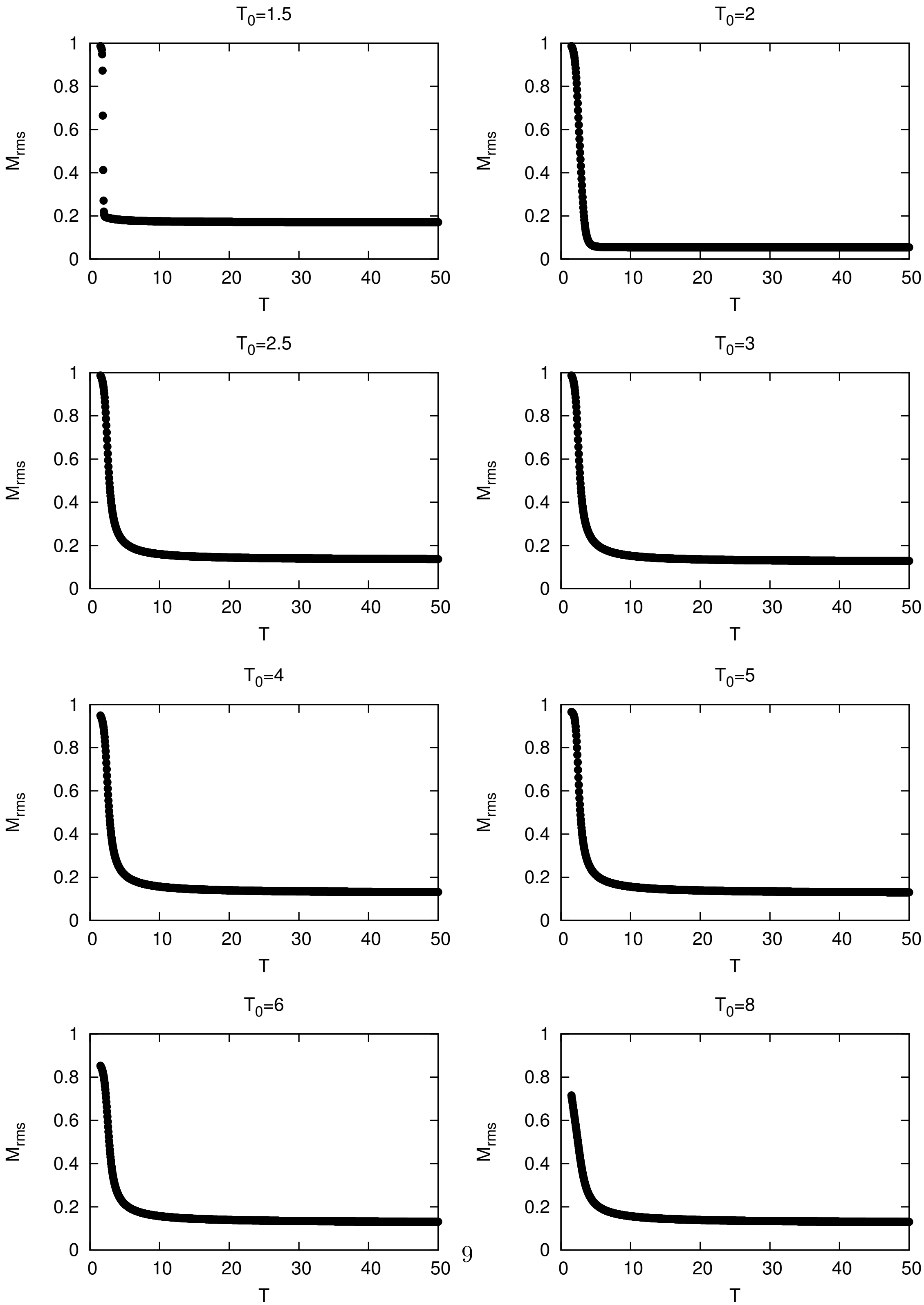

Figure 6: M_{rms} for different T_0

2.2.3 Estimate the critical temperature T_c

Onsager obtained the critical temperature for the anisotropic square lattice, when the magnetic field $h = 0$, in the thermodynamic limit,

$$T_c = \frac{2J}{k\ln(1+\sqrt{2})}$$

in reduced units,

$$T_c = \frac{2}{\ln(1+\sqrt{2})} \approx 2.269$$

For the second order phase transition, the heat capacity C_V is discontinuous close to T_c. As shown in Fig.7, C_V becomes very large close to $T \approx 2.36$. This is larger than Onsager value because the size of the lattice is very small.

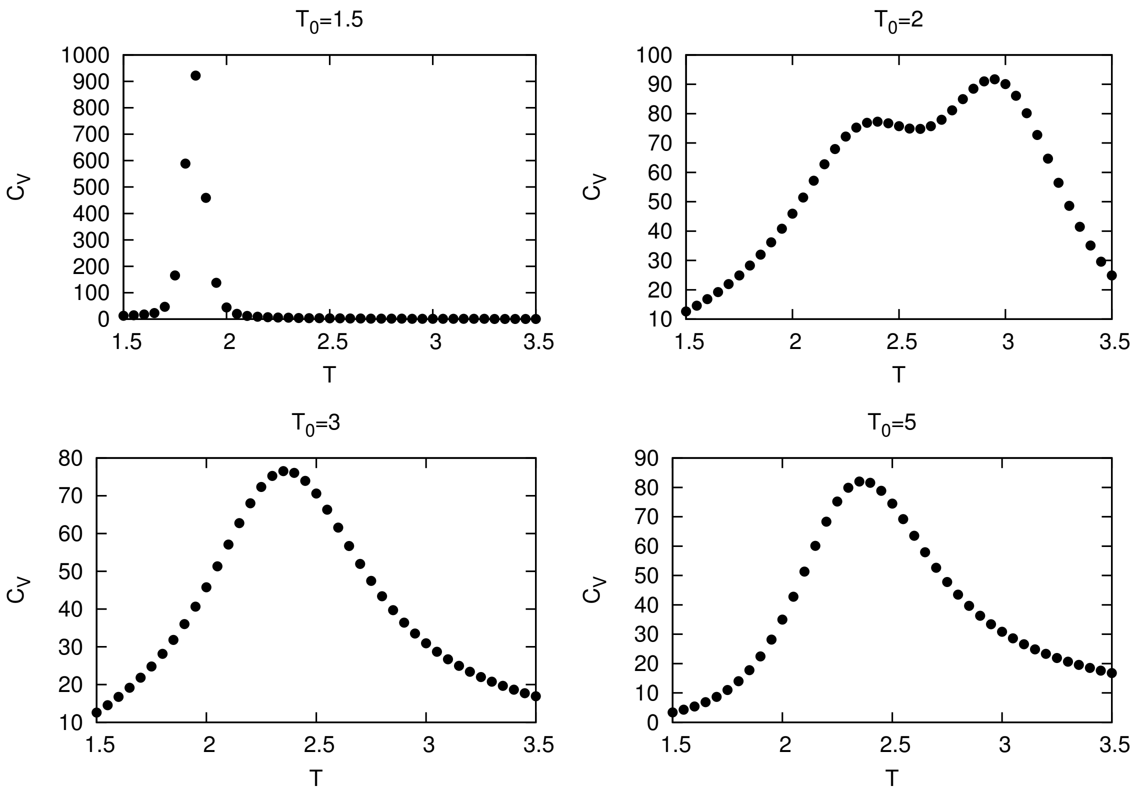

Figure 7: C_V for different T_0