Physics 514 Final Project Report

Yukai Wu

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1 Model

In this project I solve a 3-D Ising model with Monte Carlo method using Swendsen-Wang cluster update.

Consider an $L \times L \times L$ cubic lattice of classical spins $\sigma_i = \pm 1$ with Hamiltonian

$$H = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \tag{1}$$

where $\langle i, j \rangle$ means all the nearest neighbor pairs. Here periodic boundary condition is used. Let's assume $J > 0$ so the ground state has all the spins aligning in the same direction. On the other hand, at high temperature the spins tend to be random. Therefore a phase transition occurs at a temperature between these two limits. At the critical temperature, the correlation length of the system diverges as $\xi(T) \propto |T - T_c|^{-\nu}$ and the thermal dynamical quantities follow certain scaling laws. For example, specific heat, average magnetization and magnetic susceptibility scale as

$$C(T) = \frac{\langle E^2 \rangle - \langle E \rangle^2}{k_B T^2 V} \propto |T - T_c|^{-\alpha} \tag{2}$$

$$m(T) = \langle |M|/V \rangle \propto (T_c - T)^{\beta} \tag{3}$$

$$\chi(T) = \frac{\langle M^2 \rangle - \langle M \rangle^2}{k_B T V} \propto |T_c - T|^{-\gamma} \tag{4}$$

where k_B is the Boltzmann constant, E the total energy, M the total magnetization and V the system volume.

In this project I measure the critical temperature T_c and the critical exponents $\alpha, \beta, \gamma, \nu$ using Monte Carlo simulation.

2 Method

2.1 Swendsen-Wang Cluster Update

The single-spin-flip Metropolis algorithm suffers from the "critical slowing down". Because the autocorrelation time diverges as the system size increases at T_c, one need extremely large number of steps even for a relatively small system. One solution was proposed by Swendsen and Wang[1].

The Swendsen-Wang algorithm is summarized as follows:

1. Assign the bond between adjacent parallel spins as "connected" each with probability $1 - \exp(-2\beta J)$ where $\beta = 1/k_B T$. Antiparallel spins or spins that are not nearest neighbors, are never connected.
2. Use Hoshen-Kopelman algorithm[2] to identify clusters of connected spins.
3. Make measurements.
4. Each cluster is flipped independently with probability 0.5.
5. Forget about the connectivity of the spins and go back to the first step and assign "connected" bonds again.

Notice that the key point of Hoshen-Kopelman algorithm is to construct a tree structure for labels of each cluster, and the computational complexity is proportional to the depth of these trees. So every time we search the proper label (root) of a label (any node in the tree), we can change the tree structure so that all the nodes along our searching path are connected directed to the root. Therefore the next time we search the same path, less steps are needed. In this way the cluster-identifying process can be finished with time complexity $O(N) = O(L^3)$.

2.2 Finite Size Scaling

To measure the critical temperature T_c and the critical exponent ν, we can use Binder cumulant[3]:

$$U = 1 - \frac{\langle M^4 \rangle}{3\langle M^2 \rangle^2} \tag{5}$$

To the lowest order, U is independent of L at the critical temperature T_c. So if we plot U as a function of T for different L, we can determine T_c by finding where all the curves cross together. Furthermore, near T_c, the derivative of U with respect to T has the following scaling law:

$$\left.\frac{dU}{dT}\right|_{T_c} \propto L^{\frac{1}{\nu}} \tag{6}$$

This gives us a way to measure ν.

At higher accuracy, we can find that these curves for different L do not really go through the same point. For two system size L and L', the crossing point is given by[4]

$$K_{cross}(L,b) = K_c + gL^{-(w+1/\nu)}\left(\frac{b^{-w}-1}{b^{1/\nu}-1}\right) \tag{7}$$

where $K \equiv J/k_BT$ and $b \equiv L'/L$. Now if we fix the ratio b and change L, we can fit $K_{cross}(L) = K_c + aL^c$ and find the critical temperature T_c.

Once we know T_c and ν, we can choose a temperature $T \approx T_c$ such that $\xi \gg L$. Then we have

$$C(T_c, L) \propto L^{\alpha/\nu} \tag{8}$$

$$m(T_c, L) \propto L^{-\beta/\nu} \tag{9}$$

$$\chi(T_c, L) \propto L^{\gamma/\nu} \tag{10}$$

And we can calculate α, β, γ using ν we get above.

2.3 Improved Estimator

As we can see above, we need to evaluate $\langle|M|\rangle$, $\langle M\rangle$, $\langle M^2\rangle$, $\langle M^4\rangle$, $\langle E\rangle$, $\langle E^2\rangle$. We can simply calculate the exact values for the given spin configuration in each step of the Swendsen-Wang cluster update; but we can use improved estimators to evaluate the average over all possible cluster flips directly. Let's denote $\langle\rangle_{flip}$ such an average. We have

$$\langle M\rangle_{flip} = 0 \tag{11}$$

$$\langle M^2\rangle_{flip} = \sum_{cluster} S(cluster)^2 \tag{12}$$

$$\begin{aligned}
\langle M^4\rangle_{flip} &= \sum_{ijkl}\langle\sigma_i\sigma_j\sigma_k\sigma_l\rangle_{flip} && (13)\\
&= \sum_{cluster}\sum_{\substack{i,j,k,l\\ \text{in } cluster}}\langle\sigma_i\sigma_j\sigma_k\sigma_l\rangle_{flip} + 6\sum_{cluster\ A<B}\sum_{\substack{i,j \text{ in } cluster\ A\\ k,l \text{ in } cluster\ B}}\langle\sigma_i\sigma_j\sigma_k\sigma_l\rangle_{flip} && (14)\\
&= \sum_{cluster} S(cluster)^4 + 6\sum_{cluster\ A<B} S(cluster\ A)^2 S(cluster\ B)^2 && (15)\\
&= 3\langle M^2\rangle_{flip}^2 - 2\sum_{cluster} S(cluster)^4 && (16)
\end{aligned}$$

where $S(cluster)$ is the size of each cluster.

Energy is additive for bonds between nearest neighbor pairs. We can further divide such bonds into 2 classes: I. bonds within one cluster and II. bonds connecting two clusters. Because 2 spins within one cluster must be parallel to each other, while energy between spins in different clusters average to zero when we flip the clusters, we have

$$\langle E\rangle_{flip} = -J \sum_{cluster} \Big|\{\text{nearest neighbor pairs in } cluster\}\Big| \tag{17}$$

where $||$ means the number of elements in a finite set.

Similarly, when calculating E^2, there are cross terms between class I bonds which are always positive, between class I and class II bonds which average to 0, and between class II and class II bonds where only bonds pairs between the same 2 clusters are left. So finally we have

$$\langle E^2\rangle_{flip} = \langle E\rangle^2_{flip} + J^2 \sum_{cluster\ i,j} \Big|\{\text{nearest neighbor pairs between } cluster\ i \text{ and } cluster\ j\}\Big|^2 \tag{18}$$

where the summation is over all the adjacent cluster pairs.

All these improved estimators can be calculated efficiently. Unfortunately, I haven't found a way to estimate $\langle |M|\rangle_{flip}$. So it is calculated just for the given spin configuration.

3 Result

In the following, we set $J = 1$ and $k_B = 1$.

A plot of $U(T)$ for small system size $L = 6, 8, 10, 12$ is shown in Fig. 1. We can estimate $T_c \approx 4.5$

Now we can zoom in to the region close to the phase transition (by running another MC simulation), as is shown in Fig. 2. This time we get a better estimation of $T_c \approx 4.51$, and we get a rough estimation of the slopes of $U(T)$ at T_c.

As we can see, the derivative of $U(T)$ at T_c varies significantly with system size L, which suggests us to sample the temperature differently. We uniformly choose 19 points in a range of $\Delta U = 0.1$ and use the estimated slopes to sample the temperature for $L = 4, 8, 16, 32, 64$. The result is shown in Fig. 3

We can do the same calculation for $L = 3, 6, 12, 24, 48$ to get more data points for fitting. The parameters for the tangential lines at T_c are summarized in Tab. 1

Given the data of L and slope (dU/dT), we can use Eq. (6) to calculate ν, see Fig. 4. This gives us $1/\nu = 1.609 \pm 0.014$ or $\nu = 0.621 \pm 0.005$. In this report, all the uncertainty are for 95% confidence bounds.

Using data in Tab. 1, we can also calculate K_{cross}. Here we choose $b = L'/L = 0.5$. The result is summarized in Tab. 2 and then the nonlinear fitting is shown in Fig. 5. This gives us $K_c = 0.22164 \pm 0.00007$ or $T_c = 4.5118 \pm 0.0014$

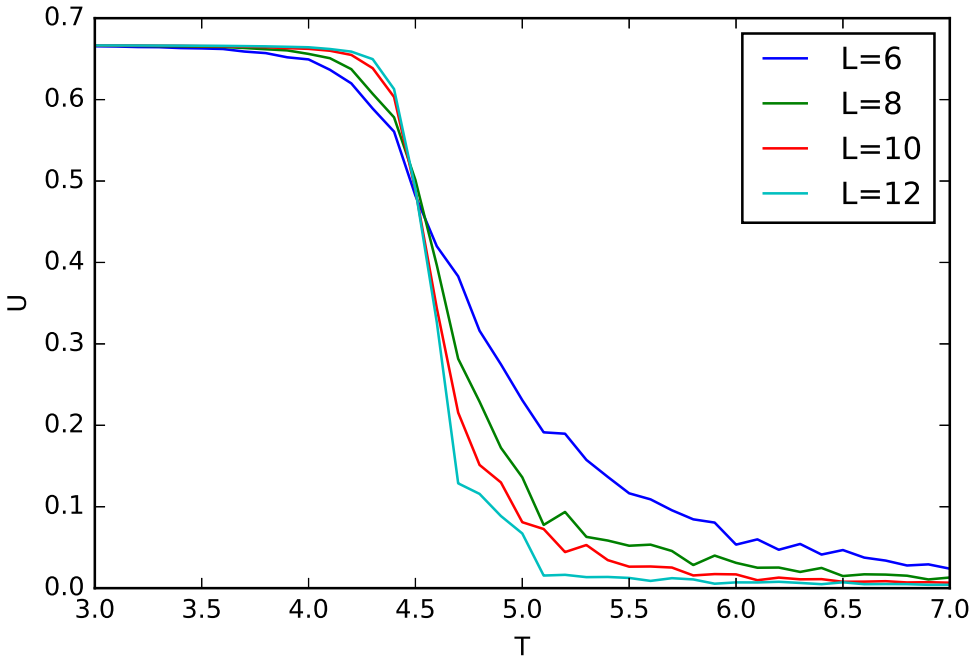


Figure 1: $U(T)$ for small system size. Here we use 1000 steps of cluster updates and the first 1/10 is used to thermalize the system.

Table 1: Slope (derivative) and intercept of tangential lines of $U(T)$ at $T \approx T_c$

L	slope k	intercept a
3	-0.180	1.312
4	-0.291	1.806
6	-0.573	3.071
8	-0.918	4.623
12	-1.768	8.452
16	-2.767	12.954
24	-5.355	24.627
32	-8.399	38.360
48	-15.822	71.852
64	-25.058	113.517

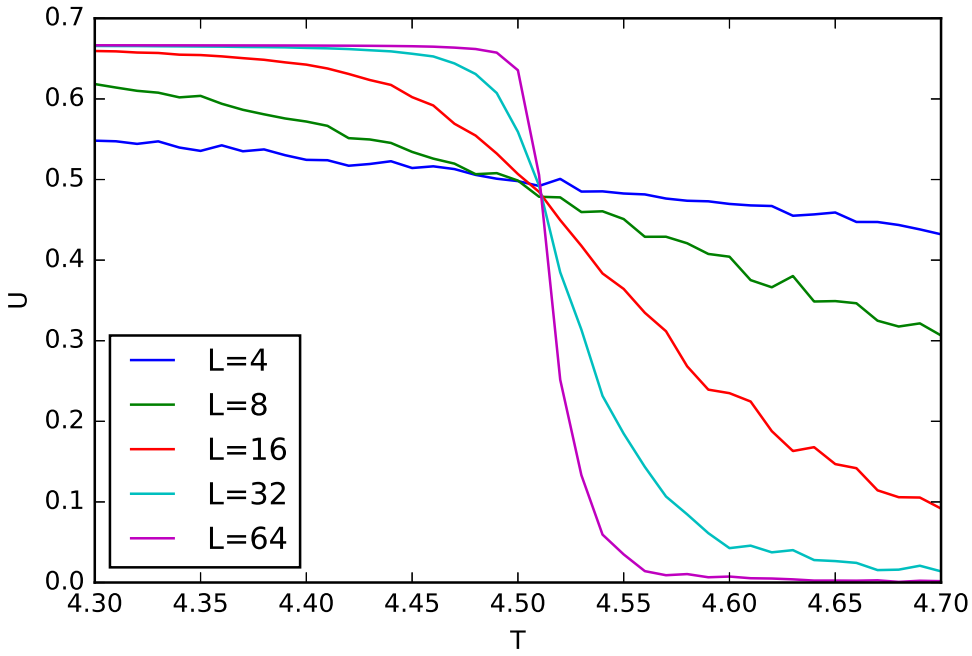


Figure 2: $U(T)$ around T_c. Here we use 10000 steps of cluster updates and the first 1/10 is used to thermalize the system.

Table 2: $K_{cross}(L, b = 0.5)$ for different L.

L	T_{cross}	K_{cross}
6	4.4758	0.22342
8	4.4928	0.22258
12	4.5029	0.22208
16	4.5057	0.22194
24	4.5093	0.22176
32	4.5110	0.22168
48	4.5118	0.22164
64	4.5115	0.22166

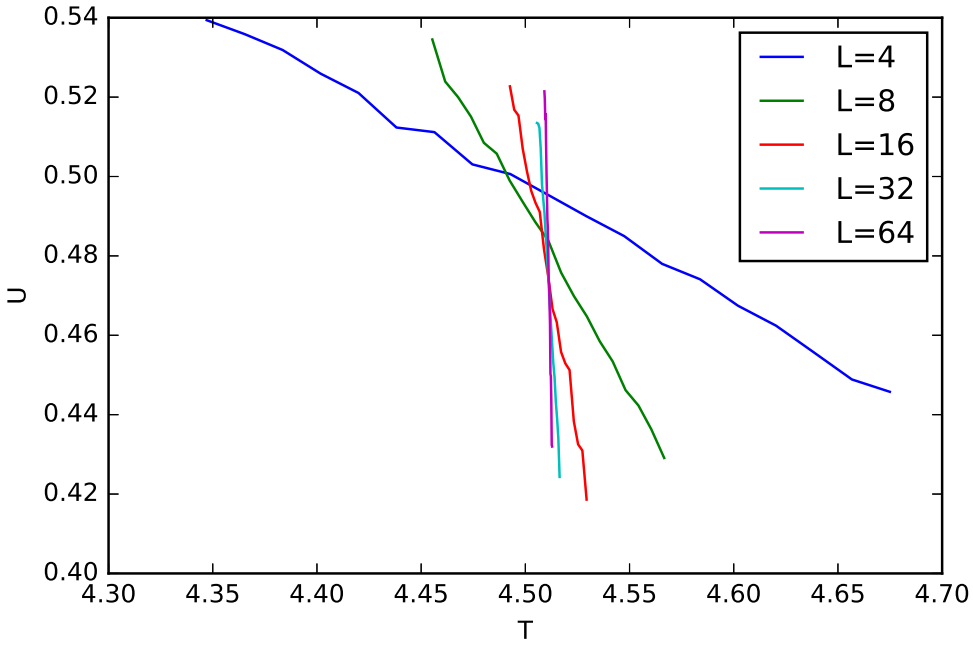


Figure 3: $U(T)$ around T_c. Here we use 100000 steps of cluster updates and the first 1/10 is used to thermalize the system.

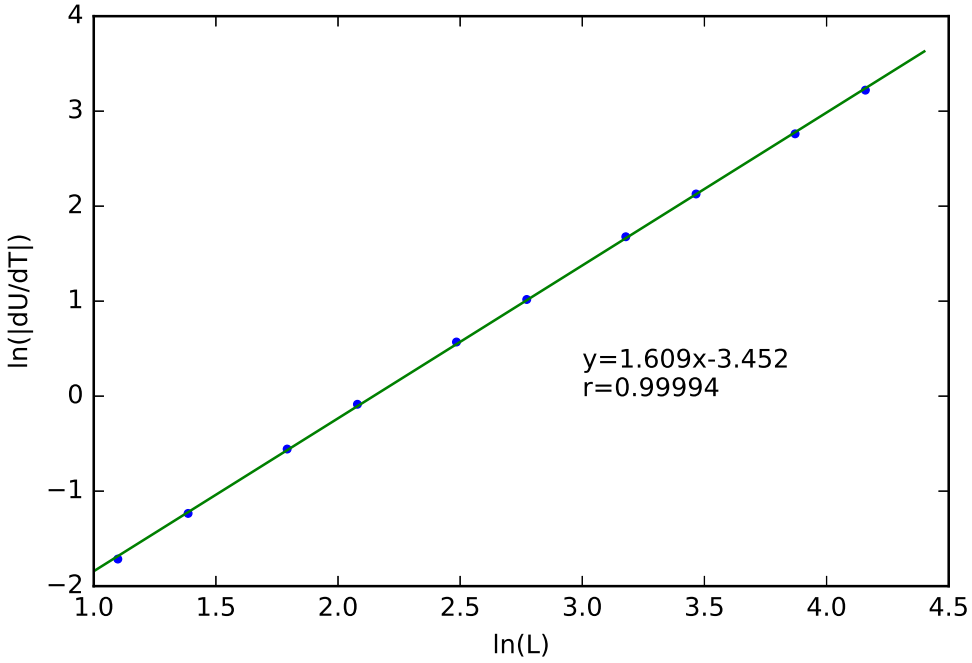


Figure 4: $\ln|dU/dT|$ around T_c v.s. $\ln L$.

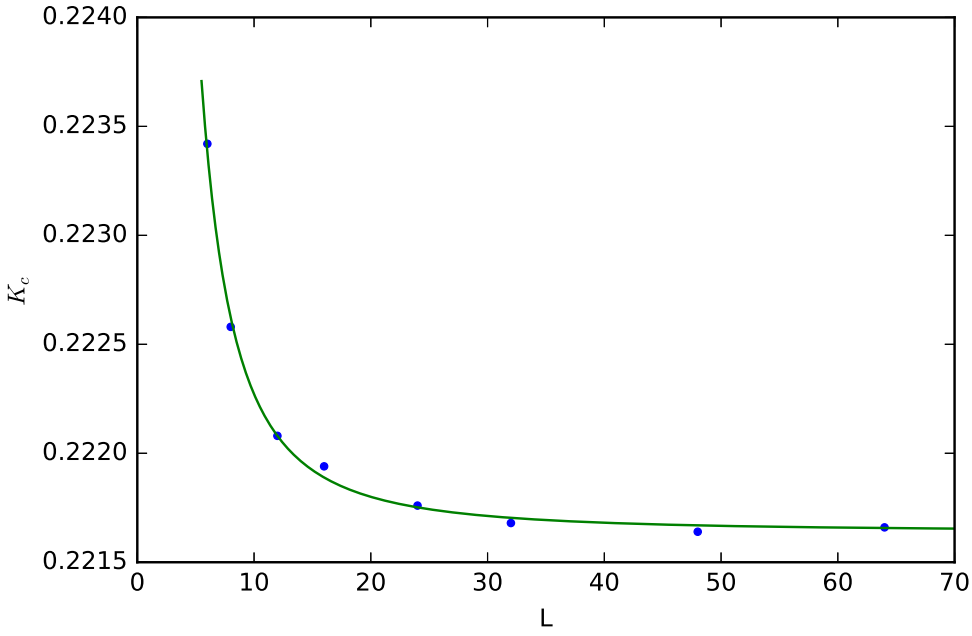
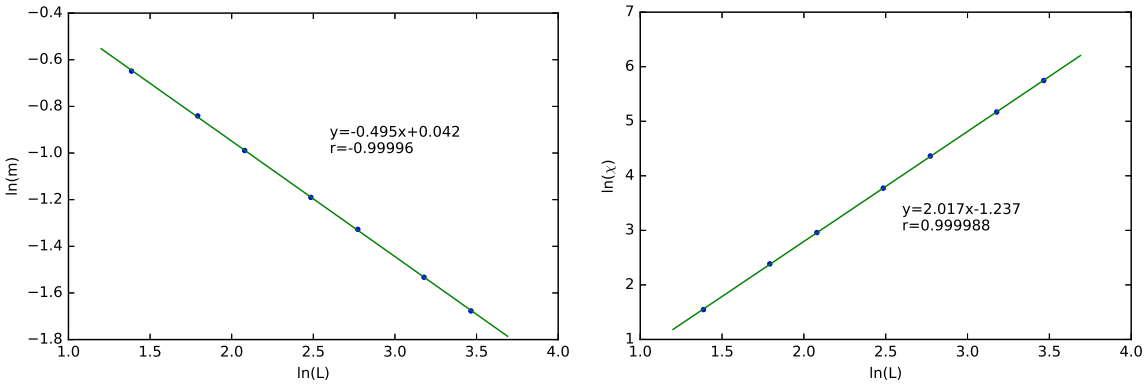


Figure 5: $K_c(L, b = 0.5)$ v.s. L.

Now we set $T = T_c$ and measure C, m and χ as functions of L. Again I use 100000 steps of cluster updates. The results of m and χ are shown in Fig. 6. This gives us $\beta/\nu = 0.495 \pm 0.005$ and $\gamma/\nu = 2.017 \pm 0.012$. And we can verify the scaling law $\gamma/\nu + 2\beta/\nu = 3.007 \approx 3 = d$.



(a) (b)

Figure 6: (a) $\ln(m)$ v.s. $\ln(L)$. (b) $\ln(\chi)$ v.s. $\ln(L)$.

However, we are not able to get α. The plot $\ln(C)$ v.s. $\ln(L)$ does not follow a linear relation, see Fig. 7. And if we blindly fit the data with linear regression, we get $\alpha/\nu \approx 0.4$ which is far from the established value $\alpha/\nu = 0.17474$. The reason is that apart from a singular term that diverges as $L^{\alpha/\nu}$, C also contains an analytical part which does not diverge as L increases[5]. And our system size is not large enough to ignore this additional term.

4 Conclusion

To sum up, in this work I use Monte Carlo simulation with Swendsen-Wang cluster update to study a 3-D Ising model. I use Binder cumulant to measure critical temperature $T_c = 4.5118 \pm 0.0014$ and critical exponent $\nu = 0.621 \pm 0.005$. Then I use finite size scaling to measure another 2 critical exponents $\beta/\nu = 0.495 \pm 0.005$ and $\gamma/\nu = 2.017 \pm 0.012$, i.e. $\beta = 0.307 \pm 0.004$ and $\gamma = 1.253 \pm 0.013$. The small difference between these values and the established values might come from higher order terms in finite size scaling or errors in Monte Carlo simulation. I also verify the scaling law $\gamma + 2\beta = d\nu$. However, I'm not able to get an accurate α from this method. I think it's because the system size is not large enough.

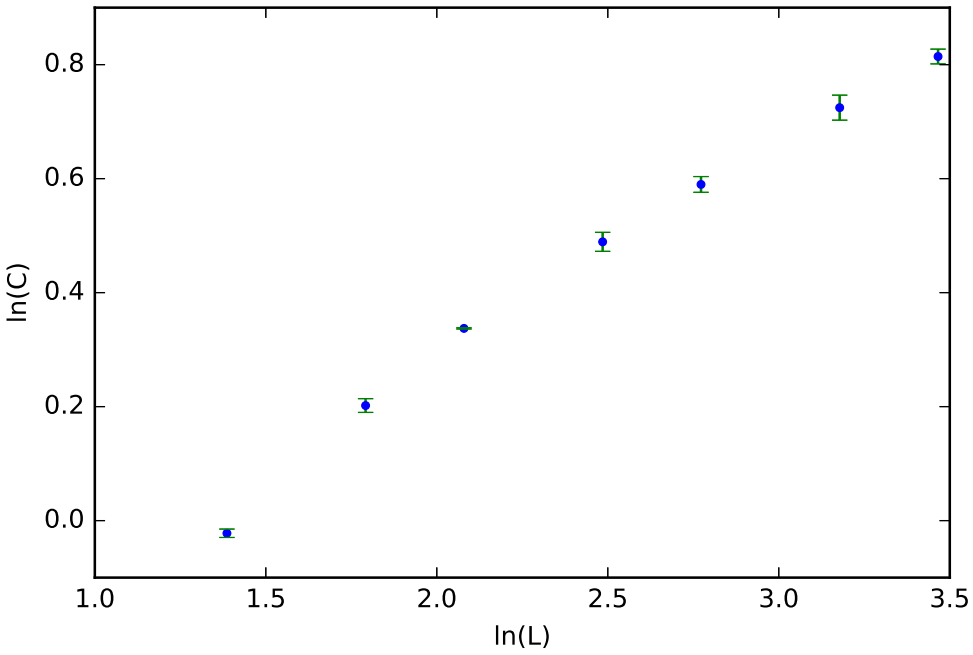


Figure 7: $\ln(C)$ v.s. $\ln(L)$. It does not follow a linear relation. The error bars are estimated by running the same simulation 3 times and finding the largest absolute difference.

References

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