Finite-Size Scaling and Critical Behavior-A Practical Review

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I will review how to extract critical behavior like critical temperature and exponents using finite-size scaling (FSS) theory. In particular, scaling behavior of these quantities and high-precision determination of critical exponents and error analysis will be demonstrated with the example of $2d$ Ising model.

I. INTRODUCTION

When dealing with data from Monte Carlo simulations, one often suffers from finite-size effects due to finite system size L. To extract the critical behavior of the system, one needs to analyze the data using finite-size scaling (FSS) theory.

Another motivation of FSS is to obtain critical exponents, which are universal and independent of the microscopic details of the system. Traditional methods like momentum shell renormalization group (RG) are often tedious and are criticized for their use of perturbative methods. FSS theory, on the other hand, provides a more straightforward way to extract critical exponents from non-perturbative numerical data.

In this review, I will discuss how to extract critical temperature and scaling exponents from the data and perform error analysis on the data. I will focus on the famously known $2d$ Ising model as an example, and show how to obtain the critical temperature T_c, scaling exponents y_t and y_h from the data, and compare them with exact values, as the $2d$ Ising model is exactly solvable.

The data are obtained from Monte Carlo simulations using standard Metropolis algorithm, with 10^6 sweep for each system size $L = 16, 32, 64, 128, 256$ and temperature point. The spacing between temperature points near the critical region is 0.005.

II. FINITE-SIZE SCALING THEORY

A. Scaling behavior of free energy

Consider the free energy $f(t, h, L^{-1})$ of a system with finite size L in d-dimensional space. Following [1], let us assume the free energy exhibits scaling behavior near the critical point T_c,

$$f_a(t, h, L^{-1}) = b^{-d} f_s(b^{y_t} t, b^{y_h} h, L^{-1} b), \tag{1}$$

where b is the size of Kadanoff spin block, $t = (T - T_c)/T_c$ and h is the external field. By assuming scaling law in this form, this amounts to only consider the singular part (with subscript s) of free energy. The difference between equation (1) and scaling law at infinite size is to add another relevant coupling L^{-1} to RG fix point with scaling dimension $d - 1$. The critical surface locates at $L = \infty$, or $L^{-1} = 0$ where the system exhibits thermodynamical limit. Now let $b = L$ we get

$$f_s(t, h, L^{-1}) = L^{-d} f_s(L^{y_t} t, L^{y_h} h, 1) := L^{-d} \mathcal{F}_s(L^{y_t} t, L^{y_h} h), \tag{2}$$

where $\mathcal{F}_s$ is a universal scaling function. It should be noted that, we scale the system with size L to size 1 by turning on the RG flow, and hence the scaling function $\mathcal{F}$ should not exhibit any singularities, as it is far away from the RG fix point.

Now one can obtain FSS behavior of various thermodynamical quantities based on f_s and its derivatives. For example,

$$m(t, L^{-1}) = L^{-d} \langle M \rangle = \left.\frac{\partial f_s}{\partial h}\right|_{h=0} = L^{y_h - d} \mathcal{M}(L^{y_t} t), \tag{3}$$

$$m'(t, L^{-1}) = T^{-2} L^{-d} (\langle EM \rangle - \langle E \rangle \langle M \rangle) = \left.\frac{\partial^2 f_s}{\partial t \partial h}\right|_{h=0} = L^{y_h + y_t - d} \mathcal{M}'(L^{y_t} t), \tag{4}$$

$$\chi(t, L^{-1}) = T^{-1} L^{-d} (\langle M^2 \rangle - \langle M \rangle^2) = \left.\frac{\partial^2 f_s}{\partial h^2}\right|_{h=0} = L^{2y_h - d} \mathcal{X}(L^{y_t} t), \tag{5}$$

$$C_V(t, L^{-1}) = T^{-2} L^{-d} (\langle E^2 \rangle - \langle E \rangle^2) = \left.\frac{\partial^2 f_s}{\partial t^2}\right|_{h=0} = L^{2y_t - d} \mathcal{C}_V(L^{y_t} t). \tag{6}$$

Where $M = \sum \sigma$ is the total magnetization and $E = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j$ is the energy. Generally speaking, the FSS behavior of these quantities can be summarized as

$$Q(t, L^{-1}) = L^{-a} \mathcal{Q}(L^b t), \tag{7}$$

where Q is some thermodynamical quantity, and $\mathcal{Q}$ is a universal scaling function.

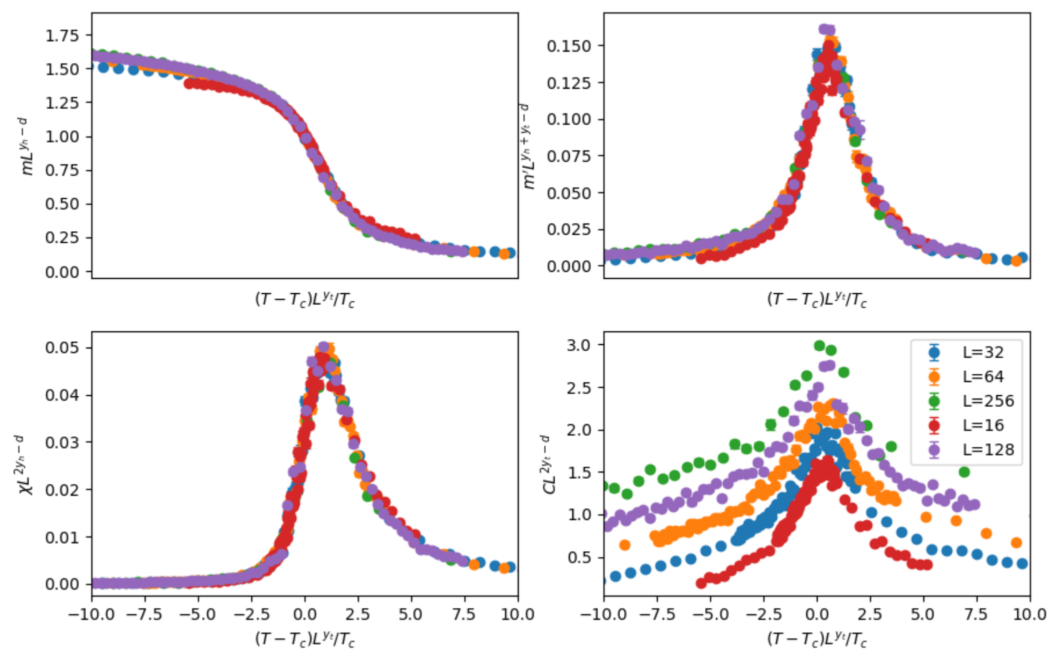

FIG. 1: Universal scaling function of thermodynamical quantities. First row: $\mathcal{M}$ and $\mathcal{M}'$. Second row: $\mathcal{X}$ and $\mathcal{C}_V$. The horizontal axis is $x = tL^{1/\nu}$. Note that for C_V, the curves do not collapse to a single curve, but shifted vertically for different L. This is because the critical exponent $\alpha = 0$ does not really reflect the singular behavior of C_V, which has a log divergence at the critical point.

In the case of $2d$ Ising model, $y_t = 1$, $y_h = 15/8$ and $T_c = 2.269$. And direct fitting of these parameters can be performed using the data obtained from Monte Carlo simulations. The fitting of m, m', χ, C_V are shown in figure 1. Note that when $x = tL^{1/\nu}$ is away from the critical region, the scaled data deviates from the universal scaling function $\mathcal{Q}$, as corrections of irrelevant couplings are not negligible.

Unfortunately, the scaling exponents y_t and y_h are unknown to us in general. In the following section, I will discuss how to extract these scaling exponents based on the FSS behavior.

B. Scaling and fitting

The FSS behavior of certain quantity Q is given by equation(7). Quantities like m', χ or C_V are of particular interests to us, as their scaling function $\mathcal{Q}$ attains a unique maximum at x_*. Thus, for a finite-size L system, the temperature $T_c(L)$ where it attains maximum satisfies $x_* = tL^{1/\nu}$. So $\nu = 1/y_t$ and T_c are fitted via

$$T_c(L) = T_c + AL^{-1/\nu}, \tag{8}$$

where A is some constant.

Instead of fitting T_c and ν directly, we first fit ν using other scaling quantities. For example, [2] the log derivative of k-th power of magnetization M^k is given by

$$\frac{\partial \ln\langle M^k\rangle}{\partial t} = T^{-2}\left(\frac{\langle M^k E\rangle}{\langle M^k\rangle} - \langle E\rangle\right) = \frac{\partial}{\partial t}\ln\left(L^{-a}\mathcal{M}^{(k)}(tL^{1/\nu})\right) = L^{1/\nu}\mathcal{M}^{(k)\prime}(tL^{1/\nu}) \tag{9}$$

and hence the maximum of such derivative is proportional to $L^{1/\nu}$. Similarly, since quantities like Binder cumulants

$$U_{2k} = 1 - \frac{\langle M^{2k}\rangle}{3\langle M^k\rangle^2} \tag{10}$$

scales as $U_{2k}(t, L^{-1}) = \mathcal{U}_{2k}(tL^{1/\nu})$, its derivative

$$\frac{\partial U_{2k}}{\partial t} = T^{-2}\left(\frac{\langle EM^{2k}\rangle - \langle E\rangle\langle M^{2k}\rangle}{\langle M^k\rangle^2} - \frac{2\langle M^{2k}\rangle}{\langle M^k\rangle^3}(\langle EM^k\rangle - \langle E\rangle\langle M^k\rangle)\right) = L^{1/\nu}\mathcal{U}'_{2k}(tL^{1/\nu}) \tag{11}$$

also scales similar to equation (9). We calculated ν based on existing data, for the estimated and error in linear regression, see figure 2.

After obtaining ν using different quantities, the final value of ν is given by the average of these values, and the error is given by the standard deviation, and resulted in $\nu = 0.998 \pm 0.018$, which is already very close to the exact value $\nu = 1$.

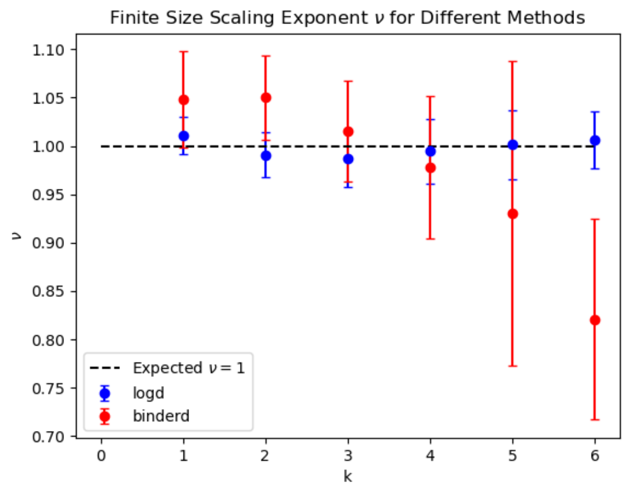

FIG. 2: Fitted ν using the log derivative and accumulate ratio U_{2k} of magnetization using different k.

For finer estimation, one can also include scaling from irrelevant couplings ω_1 as

$$\left.\frac{\partial \ln\langle M^k\rangle}{\partial t}\right|_{\max} = AL^{1/\nu}(1 + BL^{-\omega_1} + \dots) \tag{12}$$

but I will not implement this method here since the data is not sufficient for such analysis.

Now we fit the critical temperature T_c using the $T_c(L)$ in equation (8). The result using different U_{2k} and $\ln\langle M^k\rangle$ are shown in figure 3. Note that fitted T_c only behaves well for small k.

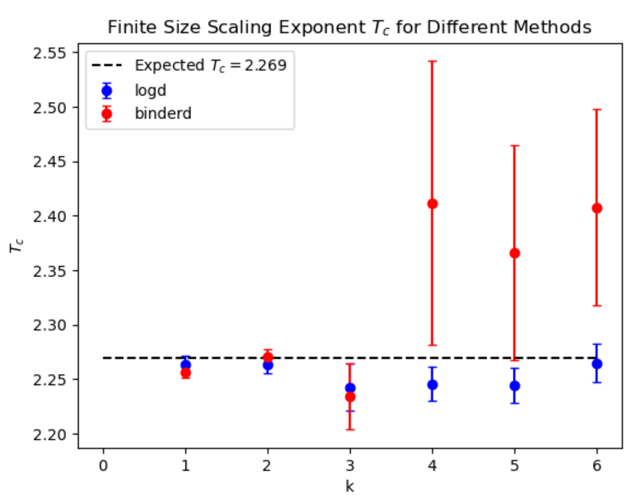

FIG. 3: Fitted critical temperature T_c using $\ln\langle M^k\rangle$ and U_{2k} for various k.

I listed fitted result using various quantities in table I. Considering the resolution of raw data is $\Delta T = 0.005$, the result we obtained is very satisfying.

Quantities	χ	C_V	U_2	U_4	ln$\langle M\rangle$	ln$\langle M^2\rangle$	exact
Fitted	2.278	2.267	2.256	2.271	2.264	2.271	2.269
Error	0.005	0.012	0.005	0.007	0.008	0.007	0.000

TABLE I: Fitted critical temperature T_c using various quantities.

Another popular method to obtain T_c is by locating the crossing of U_4 with different system size, which is based on its scaling behavior (11). However, it is hard to obtain a precise error for this method. In fact, as pointed out in [3], the crossing point of U_4 of size L_1 and L_2 also depends on the ratio L_1/L_2 and a unknown irrelevant scaling exponent ω. This makes the relation between the crossing point and T_c not straightforward, and hard to obtain a precise error.

C. Other scaling exponents

In the above section, we have obtained the critical temperature T_c and the scaling exponent $\nu = 1/y_t$. Also, one can obtain estimation of y_h from equation (3) to (6). As argued, their maximum attains a maximum $\sim L^a$, where a is linearly related to the scaling exponent y_h and y_t. This allow us to restrict the value of y_h and y_t. See figure 4 for these bounds on the y_t-y_h plane.

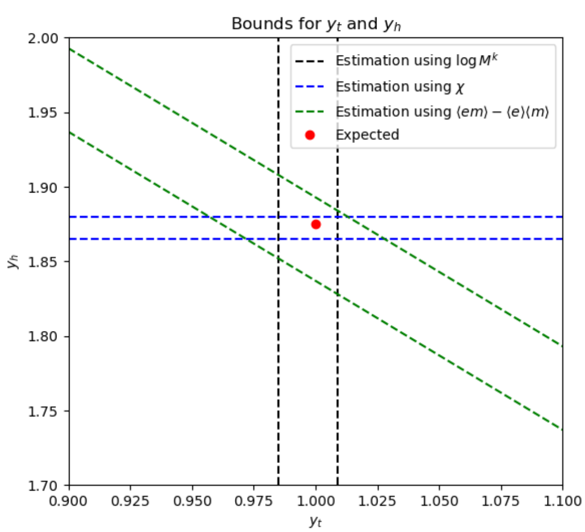

FIG. 4: Restricted region of y_h and y_t based on the maximum of χ, m', ln$\langle M^k\rangle$.

It is possible to get further estimation of y_h and y_t by taking derivative of existing quantities. However, these quantities contains higher momentum of existing data, and hence the error of these quantities tends to be larger for small scale data, as seen in previous discuss of $\ln\langle M^k\rangle$ and U_{2k}.

D. Other fitting method

As seen above, we have used the finite-size scaling hypothesis to obtain the critical exponents. The main method is to fit the data based on its maximum value. There are also other methods to obtain the scaling exponents. For example, one can [4] fit the whole curve of quantity Q based on the scaling hypothesis (7) directly, this allow us to fully utilize the data obtained. The drawback of this method is that it is hard to obtain the error of the fitted parameters, as the fitting is highly nonlinear. Also it requires a raw data in good quality, as the fitting is sensitive to the noise in these data. And hence these method are not popular in practice.

III. ERROR ANALYSIS

Now I follow [3, 5] to analyze the error of Monte Carlo simulations. The process is as follows:

1. For collected data $(x_1, \ldots, x_N)$, divide it into n blocks $J_1, \ldots, J_n$, with each block containing $N_b = N/n$ data points. The ith Jackknife block is given by deleting those data in the J_i block. That is, each Jackknife block contains $N_b(n-1)$ data. Here N_b should be much larger than the autocorrelation length of the data:

$$\tau = \frac{1}{2} + \sum_{k=1}^{k_{\text{max}}} C_{\text{auto}}(k), \quad C_{\text{auto}}(k) = \frac{1}{N-k}\sum_{i=1}^{N-k}(x_i - \bar{x})(x_{i+k} - \bar{x}), \tag{13}$$

   where k_{max} is the smallest k such that $C_{\text{auto}}(k) < 0$, that is, the autocorrelation is fluctuation dominated. In practice, one use $N_b = 6\tau$ as $e^{-6} < 0.003$.

2. Evaluate quantity f based on these Jackknife block $y_i^J = f(x_k)_{k\notin J_i}$, The average of given quantity f is then given by the average of all Jackknife blocks $\bar{y}^J = \frac{1}{n}\sum_{i=1}^{n} y_i^J$, while the

variance is given by

$$\sigma^2 = \frac{n-1}{n}\sum_{i=1}^{n}(y_i^J - \bar{y}^J)^2.$$

Note that here, we assume the data is uncorrelated, which is indeed the case for our data. The maximum of C_V and χ are located at different temperature points, even with same system size L. This originates from the fact that the amplitude A in equation (8) changes with respect to different quantity. As mentioned, the Monte Carlo simulations are performed independently for each temperature point. However for other approaches using different sampling methods [2, 3], the underlying data may be correlated, and the error analysis should be performed accordingly.

IV. CONCLUSION

In this review, I have discussed how to extract critical temperature and scaling exponents from the data using finite-size scaling theory. I have also discussed how to perform error analysis on the data using Jackknife method. The results are compared with exact values, and the error is estimated based on the Jackknife method.

The code to perform the monte carlo simulation and data analysis are available here.

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