NUMERICAL STUDY OF FINITE SIZE SCALING FOR FIRST ORDER PHASE TRANSITIONS

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ABSTRACT

I present results of simulations of the $q=10$ and $q=20$ 2-d Potts models in the transition region. The asymptotic finite size behavior sets in only for extremely large lattices. We learn from this simulation that finite size scaling cannot be used to decide that a transition is first order.

Keywords: First Order Phase Transitions; Monte Carlo.

1. Introduction

This talk addresses the question of deciding whether a transition is first order or not, using Monte Carlo simulations.

• Very strong transitions are easy to detect. The system behavior is very close to the infinite volume behavior. Ergodicity is broken. Thermodynamical quantities are discontinuous at the transition point, with metastable branches. A starting configuration half ordered, half disordered will relax to very different states on both sides of the transition.

With extreme statistics, one is able to sample the coexisting phases (although this may be forbiddingly costly). The time evolution of any thermodynamical quantity then shows flip-flops between the phases, and the corresponding probability distribution is made of well separated peaks.

• In less clear cases, one must simulate systems of increasing volumes $L^d$ and try to convince oneself that the above described very large volume behavior is approached. Let me use the language of energy driven transitions in what follows, and introduce the energy probability distribution $P_L(E)$. In the transition region, it has two peaks of heights $P_L^o$ and $P_L^d$, separated by a minimum of height $P_L^{min}$.

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For a first order transition, at fixed $P_L^d/P_L^r$, one has

$$\frac{1}{L^d} \ln \frac{P_{\text{min}}^L}{P_0^L} \to 0 \quad L \to \infty$$

This has been proposed by Lee and Kosterlitz 1 as an indicator of first order phase transitions (see also 2 3).

Another class of indicators are moments of the distribution $P_L(E)$, that goes to zero in the large volume limit, for all temperatures, but at a first order transition point. An example is the energy fluctuation $CV/L^d = \beta^2(<E^2>-<E>^2)$, another is Binder’s famous cumulant $BL = \frac{1}{3}(1-<E^4>/<E^2>^2)$. One can also plainly look at a plot of $P_L(E)$ and decide “by eyes” whether it approaches two delta functions as $L$ grows.

• The most sophisticated (and trustworthy) method is finite size scaling. One insist in seeing the finite size behavior as predicted by the theory in the vicinity of a first order phase transition. In that case only can one be pretty sure that the trend observed for lattices of increasing sizes does continue up to the thermodynamical limit. One insist on seeing

$$\frac{1}{L^d} \ln \frac{P_{\text{min}}(L)}{P_0(L)} \sim A/L$$

$$CV_{\text{max}}/L^d \sim CV^{(1)} + CV^{(2)}/L^d$$

where $CV_{\text{max}}$ is the maximum of the specific heat,

$$BL_{\text{min}}/L^d \sim BL^{(1)} + BL^{(2)}/L^d$$

where $BL_{\text{min}}$ is the minimum of $BL$

My interest in first order phase transitions started with the 1988-1989 controversy over the order of the deconfinement phase transition of pure SU(3) gauge theory, and the question whether some modified 3-d Z(3) Potts model has a first order transition or not. Our data 4 were very convincing showing that $BL_{\text{min}}$ has a non zero large volume limit, however we did not observe the predicted $1/L^3$ finite size behavior (our data behave nearly like $1/L^2$). This led us to investigate the 2-d q=10 Potts model, as an example of a model with a strong first order transition, searching for the predicted finite size behavior.

2. Exact Results

Those have been obtained 5 for models that can be represented by a contour expansion with small activities, like 6 the q states Potts model for large q. In such a case, the partition function for a $L^d$ lattice with periodic boundary conditions can be written as

$$Z(\beta, L) = e^{-L^d\beta f_d(\beta)} + q e^{-L^d\beta f_u(\beta)} + \mathcal{O}(e^{-bL})e^{-\beta f(\beta)L^d} \quad ; \quad b > 0 \quad (2.1)$$
where \( f_o(\beta) \) and \( f_d(\beta) \) are smooth \( L \) independent functions. The free energy is 
\[
f(\beta) = \min\{f_o(\beta), f_d(\beta)\}.
\]
The phenomenological two gaussian peak model of the energy probability distribution \( P_L(E) \) introduced by K. Binder and D. Landau 7,8 follows through inverse Laplace transform. The above exact result fixes the relative weights of the two peaks: At the infinite volume limit transition point, \( \beta = \beta_t \), the ordered and disordered peak weights are exactly in the ratio \( q \) to one.

The two gaussian peak model is not however a good representation of \( P_L(E) \) for all \( E \)’s. It fails to describe the region between the two peaks, and does not account for the observed \( L \) dependence of the position of the two maxima of \( P_L(E) \) when \( \beta = \beta_t \). This would require the understanding of the correction term in Eq.( 2.1.)

To the order in \( 1/L^d \) we consider, all quantities are expressed in terms of \( \beta_t \) and of the energies and specific heats of the two coexisting phases. The transition temperature, \( E_o, E_d \) and the difference \( C_o - C_d \) are known exactly for the 2-d Potts models 9. It follows from Eq.( 2.1) that the specific heat
\[
CV = \beta^2 L^d(<E^2> - <E>^2)
\]
has a maximum at
\[
\beta(CV_{\text{max}}) = \beta_t - \frac{\ln q}{E_d - E_o} \frac{1}{L^d} + \frac{\beta^2_{CV}}{L^{2d}} + O(1/L^{3d}).
\]
The height of this maximum increases linearly with \( L^d \)
\[
CV_{\text{max}} = L^d \frac{\beta^2}{4} (E_o - E_d)^2 + CV^{(2)} + O(1/L^d).
\]
whereas for fixed \( \beta \neq \beta_t, CV(\beta) \) goes to a constant, as \( L \) goes to infinity. One finds that \( BL \) reaches a minimum equal to 10,5,11
\[
BL_{\text{min}} = -\frac{(E_o^2 - E_d^2)^2}{12(E_o E_d)^2} + \frac{BL^{(2)}}{L^d} + O(1/L^{2d})
\]
at the point
\[
\beta(BL_{\text{min}}) = \beta_t - \frac{\ln(q(E_o/E_d)^2)}{E_d - E_o} \frac{1}{L^d} + \frac{\beta^2_{BL}}{L^{2d}} + O(1/L^{3d}).
\]

Expressions of the coefficients \( \beta^2_{BL}, BL^{(2)}, \beta^2_{CV} \) and \( CV^{(2)} \) as functions of the \( E_i \)’s and \( C_i \)’s can be found in 11. Although the use of \( BL_{\text{min}} \) as an indicator of the order of phase transitions has been much publicized, \( CV_{\text{max}}/L^d \) is as good an indicator indeed. The value of \( BL \) depends on the choice made of the arbitrary constant one can add to the definition of the energy, this leads to introduce the quantity 12
\[
U_4 = \frac{<(E - <E>)^4>}{<(E - <E>)^2>^2}.
\]
which is independent of such a constant. $U_4$ is strictly larger than one, but at a first order transition point, in the infinite volume limit. For large but finite volumes, $U_4$ reaches a minimum

$$U_{4\text{min}} = 1 + \frac{8(C_o + C_d)}{L^d \beta_t^2 (E_o - E_d)^2} + O(1/L^d).$$

at the point

$$\beta(U_{4\text{min}}) = \beta_t - \frac{\ln(q)}{E_d - E_o} + \frac{(C_o - C_d)(\ln^2(q) - 8)}{L^d \beta_t^2 (E_o - E_d)^3} + O(1/L^d).$$

$BL_{\text{min}}$ (or $CV_{\text{max}}/L^d$) and $U_{4\text{min}}$ are dual since $BL_{\text{min}}$ (or $CV_{\text{max}}/L^d$) going to zero means second (or higher order), whereas $U_{4\text{min}}$ going to one means first order.

The above formulae for the extrema $CV_{\text{max}}$, $BL_{\text{min}}$, $U_{4\text{min}}$ and the corresponding effective $\beta$’s have higher power law corrections that may hide the asymptotic behavior on lattices that can be simulated. In contrast, the expressions for bulk averages evaluated at the (infinite volume limit) transition point $\beta = \beta_t$ do not have power law corrections, as a consequence of Eq.2.1. The average energy is given by

$$E(\beta_t) = \frac{E_d + qE_o}{1 + q} + O(e^{-bL})$$

and the value of the specific heat is

$$CV(\beta_t) = \frac{C_d + C_o q}{1 + q} + \frac{L^d q}{(1 + q)^2} (E_o - E_d)^2 \beta_t^2 + O(e^{-bL})$$

The energy at $\beta_t$ does not depend on the lattice size, up to exponentially small corrections. This provides an efficient estimator of the transition temperature 6,13 by the following “two-lattice method”. One simulates lattices of increasing sizes $L_1 < L_2 < L_3 < \ldots$, and consider $\beta_{\text{eff}}(L_i, L_{i+1})$, the solution of the fixed point equation

$$E_{L_i}(\beta) = E_{L_{i+1}}(\beta)$$

for $i = 1, 2, \ldots$. The estimate $\beta_{\text{eff}}(L_i, L_{i+1})$ converges towards $\beta_t$ with exponential pace. The spectral density (a.k.a Ferrenberg-Swendsen FS, or reweighting) method is invaluable for locating extrema and zeros with Monte Carlo data as input. It allows to reconstruct the value of a thermodynamical average for any $\beta$ from one run performed at a given $\beta_{\text{M.C.}}$ in the vicinity of the transition. It is well known that this method has problems close to a second order point. With moderate statistics, it predicts extraneous extreme for e.g. the specific heat 15. This never occurred to us with first order points.

To summarize, the extrema of $CV_{\text{max}}/L^d$, $BL_{\text{min}}$, and $U_{4\text{min}}$ behave in the large volume limit like $X^1 + X^2/L^d + O(1/L^d)$, $CV(\beta_t)$ behaves like $X^1 + X^2/L^d + $
\(O(e^{-bL})\). The four different constants \{X^1\} are exactly known. One single unknown parameter, e.g. the ordered specific heats \(C_o\), fixes the four \(X^2\)'s.

3. Simulation of the q=10 model

We have performed a \(\approx\) 800 CRAY X-MP hours simulation of the \(q = 10\) 2-d Potts model, in order to determine how large \(L\) has to be in order to see the asymptotic regime described in 5. This is a model with a strong, obvious, first order transition, with \(16\) a correlation length \(\xi(\beta^*) \sim 6\). The precision of our data is better by more than one order of magnitude than in 8. We have compared our results for the extrema of \(CV/L^d, BL\) and \(U_4\), and for the value \(CV(\beta_i)\) with the large volume predictions.

We simulated lattices up to \(L = 50\) (where the autocorrelation times are \(\tau_S \approx .9 \times 10^6\) and \(\tau_{NS} \approx 2.5 \times 10^6\)). For all four quantities, we see deviations from the \(X^1 + X^2/L^d\) limiting behavior. There is nothing to worry about that, it only means that our precision is good. Really disturbing however, is that these corrections do not seem to behave simply as function of \(L\), and are definitely not under control. The values for the four slopes \(\{X^2\}\) one would infer from our data give inconsistent estimates of \(C_o\). Three possible explanations are i) Eq.( 2.1) is only proven in the large \(q\) limit, it may not hold down to \(q = 10\). ii) Much larger lattices may be needed in order to extract the true asymptotic behavior, although in our data \(P_L(E)\) has a textbook first order shape. iii) A programming error is always possible.

Before doing the simulation, we hoped that \(CV(\beta_i)\) would be asymptotic earlier than \(CV_{max}\), since corrections are \(O(e^{-bL})\). The data do not substantiate this hope, \(CV(\beta_i)\) has larger error bars, but does not seem to reach its asymptotic behavior earlier. Note that the estimate of \(C_o\) we get from \(CV(\beta_i)\) is much higher than the others.

4. Simulation of the q=20 model using the Multicanonical Algorithm

The conventional Metropolis (and Swendsen-Wang 17) algorithm suffers from exponential slowing down. This makes simulations on lattices much larger than used to day, impossible even with vastly more powerful computers. It has been proposed by B. Berg and T. Neuhaus 18 to perform the simulation with an Hamiltonian designed in such a way that \(P_L(E)\) is very smooth between \(E_o\) and \(E_d\), and to reweight the events when computing expectation values. The new “multicanonical” algorithm has only polynomial slowing down.

We 19 used this algorithm in order to simulate the q=20 Potts model. It has a stronger first order transition and a smaller correlation length than the q=10 model. This means that the large volume regime sets in for smaller lattices for \(q = 20\) than for \(q = 10\). We ran mainly on IBM RS6000 workstations, and simulated lattices as large as \(38^2\). In contrast with the \(q=10\) case, the values of the four slopes \(\{X^2\}\) one infer from our data give consistent estimates of \(C_o\). As an example, Fig1 gives our results for \(CV_{max}/L^d\) together with the theoretical estimate using the value \(C_o = 5.2 \pm .2\), and Fig2 gives our results for \(CV(\beta_i)\) together with the theoretical
estimate using the same value for $C_o$. Note that $CV(\beta_1)$, reaches its asymptotic behavior much earlier than $CV_{max}$, as predicted by the theory. In conclusion the asymptotic behavior predicted by K. Binder, and later proven by C. Borgs and R. Kotecký only sets in for very large lattices. The lattice size must fulfil the conditions $L >> \xi$, $L^{d-1} >> 1/A^{od}$ where $A^{od}$ is the order-disorder surface tension (If Widom’s relation 20 holds this condition is equivalent to the first one), and $L^d >> C_o/(E_o - E_d)$, $L^d >> C_d/(E_o - E_d)$, where $>>$ means five to ten times larger. It is unfortunate that for such large systems, the transition is blatantly first order.

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Figure 1: $CV_{max}/L^2$ as a function of $1/L^2$ for the 2-d q=20 Potts model.
Figure 2: $BL_{\text{min}}/L^2$ as a function of $1/L^2$ for the 2-d $q=20$ Potts model.

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