Advanced Statistical Physics
Homework: Finite Size Scaling

October 2021

This homework investigates the use of the finite size scaling technique to identify the phase transition and critical behaviour in systems with continuous phase transitions. It has two parts. One concerns analysis of data of the Ising model, and the second one deals with the analytic treatment of a stochastic model.

1 The Ising model

We will apply the finite size scaling technique to analyse numerical Monte Carlo data for the Ising model

$$H(\{s_i\}) = -J \sum_{\langle ij \rangle} s_i s_i - h \sum_i s_i \equiv H_J(\{s_i\}) + H_h(\{s_i\}) \tag{1}$$

defined on two and three dimensional lattices. The spin variables are $s_i = \pm 1$ for all i, the ferromagnetic coupling constant is $J > 0$ and h is a uniform magnetic field. The sum $\sum_{\langle ij \rangle}$ runs over nearest neighbours on the lattices, which have linear sizes L. The convention used for the definition of this sum will be inferred from the data. The system is in equilibrium with a thermal bath at inverse temperature $\beta = 1/(k_B T)$. We have defined the two contributions to the Hamiltonian, $H_J(\{s_i\})$ from the two-body coupling, and $H_h(\{s_i\})$ from the magnetic field contribution, for later convenience.

2 The data

The data in `www.lpthe.jussieu.fr/~leticia/TEACHING/ICFP/Homework` have been produced by M. Picco (LPTHE) using the Swendsen-Wang (two dimensional) and Wolf (three dimensional) cluster algorithms which allow one to speed up the Monte Carlo simulations close to the critical point, and equilibrate samples of much larger sizes than the single spin flip Monte Carlo codes. In the following we measure temperature in units of J or, equivalently, we set $J = 1$.

The representation used is such that H has been multiplied by β.

The three first files have data for

The 2dIM at different	T and $h = 0$	OUT2dL#Th0
The 2dIM at different	h and $T = T_c$	OUT2dL#T$_c$
The 3dIM at different	T and $h = 0$	OUT3dL#Th0

The label # close to L means that the values of the system sizes, L, are placed there in the names of the files. OUT3dL4Th0 contains data for the three dimensional Ising model with linear size $L = 4$, at various temperatures, and under no applied magnetic field. OUT2dL4Tc contains data for the two dimensional Ising model with linear size $L = 4$, at the critical temperature, and under different applied fields. The columns are organised as

$$L \qquad 1/\beta \qquad h \qquad m \qquad -e \qquad L^2\sigma_m^2 \qquad L^2\sigma_H^2 \qquad \#\,\text{samples} \tag{2}$$

in the two dimensional case at $h = 0$ (file OUT2dL#Th0)

$$L \qquad 1/\beta \qquad h \qquad m \qquad -e_J \qquad -e \qquad \sigma_m^2 \qquad L^2\sigma_{H_J}^2 \qquad L^2\sigma_H^2 \qquad \#\,\text{samples} \tag{3}$$

in the two dimensional case at T_c (file OUT2dL#T$_c$) and

$$L \qquad 1/\beta \qquad h \qquad m \qquad m2 \qquad -e \qquad e2 \qquad \sigma_{H_J}^2 \qquad \sigma_H^2 \qquad \#\ \text{samples} \tag{4}$$

in the three dimensional case at $h = 0$ (file OUT3dL#Th0) with

$$\begin{aligned}
m &= \frac{1}{L^d}\left\langle \left| \sum_i s_i \right| \right\rangle & m2 &= \left\langle \left(\frac{1}{L^d} \sum_i s_i \right)^2 \right\rangle \\
\sigma_m^2 &= m2 - m^2 \\
e_J &= \frac{1}{L^d}\langle H_J(\{s_i\})\rangle & e &= \frac{1}{L^d}\langle H(\{s_i\})\rangle \\
e2 &= \frac{1}{L^{2d}}\left\langle (H(\{s_i\}))^2 \right\rangle & e_J2 &= \frac{1}{L^{2d}}\left\langle (H_J(\{s_i\}))^2 \right\rangle \\
\sigma_H^2 &= e2 - e^2 & \sigma_{H_J}^2 &= e_J2 - e_J^2
\end{aligned} \tag{5}$$

samples gives the number of samples used to calculate the averages.

2.1 Questions

We start with a series of general questions. Justify your answers.

1. Can the free-energy of a finite size system be non-analytic?
2. Do you expect the actual critical temperature of a finite dimensional system to be higher or lower than the one found with the mean-field approximation?
3. Which is the relation between the fluctuations of the magnetisation and the linear magnetic susceptibility? Write it down.
4. Which is the relation between the fluctuations of the energy and the heat capacity? Write it down.

We now perform the data analysis.

1. Use the information about the energy density given in the data-files to deduce which is the convention for the sum over nearest-neighbours on the lattice, $\sum_{\langle ij\rangle}$, used.

2. Using the data in the files, make two plots of the magnetisation density m as a function of temperature, for the $2d$ and $3d$ Ising models in the absence of magnetic field and different values of the linear size L. Discuss these curves. Write down the equation that determines the mean-field magnetisation density (for the sum convention identified in the previous item) and trace the solutions on the same plots. In which case is it closer to the numerical data in finite d? You can quantify the answer to this question calculating $T_c^{\mathrm{MF}}/T_c - 1$. Why?
3. In the $d = 2$ case, find in the literature Onsager's expression for m and trace it in the same plot. Compare to the numerical data.
4. One can determine the ratio exponent β/ν from the relation $\langle m2\rangle^{1/2}(T_c) \sim L^{-\beta/\nu}$. Plot $\langle m2\rangle^{1/2}$ as a function of temperature.
   Determine from Onsager's exact expression for m the exponent β in $d = 2$. Compare to what you found with the data analysis, setting $\nu = 1$.
5. Make the scaling plots for the magnetisation densities in the $2d$ and $3d$ dimensional cases. In the bidimensional case work with the distance from the critical point, $t \equiv (T - T_c)/T_c$ with no absolute value, while in the three dimensional case use $|t|$ to build the scaling variable.
6. Consider now the applied field dependence of the magnetisation in the Ising model in $d = 2$. Confront the numerical data for $m(h)$ to the mean-field predictions and to Onsager's result. Which one represents better the data? Think about using a double logarithmic representation to make the algebraic dependence easy to visualise.
7. Make plots of the linear magnetic susceptibility in the $2d$ model using the data in OUT2dL#Th0. Do you see the expected qualitative behaviour?
   Imagine that the maximum value in this plot scales as
   $$\chi_{\max}(L) \propto (\beta_c(L) - \beta_c(L \to \infty))^{-\gamma} \propto L^{\gamma/\nu} \tag{6}$$
   where $\beta_c(L \to \infty)$ is here a fitting parameter to be later compared to Onsager's exact value. Proceed as follows:
   (a) Apply some smoothing of this data (e.g. with gnuplot, the "smooth bezier" option to the "plot" command).
   (b) Estimate the pair $(\beta_c(L), \chi_{\max}(L))$ for each L, where $\beta_c(L)$ is the position of the maximum and $\chi_{\max}(L)$ the height at the maximum.
   (c) Make a power law fit of the maximum location $\beta_c(L) = \beta_c(L \to \infty) - cL^{-1/\nu}$. This is a three parameter fit, $\beta_c(L \to \infty)$, c, ν, and serves to find estimates for the infinite size β_c and the exponent ν.
   (d) Get γ from $\chi_{\max} \sim L^{\gamma/\nu}$.
   (e) Compare all values from to Onsager's exact ones.
8. Use now the more detailed data in the critical region that you can find in the files called OUTL#h0close. Do you find improved results? What does this teach you?
9. How would you exploit the data in the files to find the exponent α?

3 The Galton-Watson model

Sharp changes in the behaviour of a system not only arise in the thermodynamic equilibrium of infinite size systems. Dynamic phase transitions are also of interest. The concepts and ideas learnt in the equilibrium case can sometimes be transposed and applied in the new contexts. In this Section we will study one model with this occurs, paying special attention to finite size effects, the theme of this Homework.

Bienaymé on the one hand, and Galton and Watson on the other, analysed a stochastic process, more than one hundred years ago, to study the extinction of (prominent) families [1].

Consider elements (say, mothers) who give rise to other elements (say, daughters). The Galton-Watson process assumes that each of these elements triggers a random number K of offspring elements in each generation. The Ks are independent identically distributed (*i.i.d.*) random variables, with probabilities

$$P(K=0) = p_0, \qquad P(K=1) = p_1, \qquad \ldots, \qquad P(K=k) = p_k, \qquad \ldots \tag{7}$$

with $k = 0,1,\ldots,\infty$. The probabilities are normalised, $\sum_{k=1}^{\infty} p_k = 1$. An example of a Galton-Watson tree is shown in Fig. 1.

In the zeroth generation of the process there is a single element, and the number of elements at this step is $Z_0 = 1$. The K offsprings of this first element constitute the first generation. The number of elements in this first generation is called Z_1. The definition of the probability P implies that $P(Z_1 = k) = p_k$. The number of elements in the tth generation is called Z_t. t is playing the role of a discrete time and Z_t is a random variable in its turn, with distribution determined by $P(K)$.

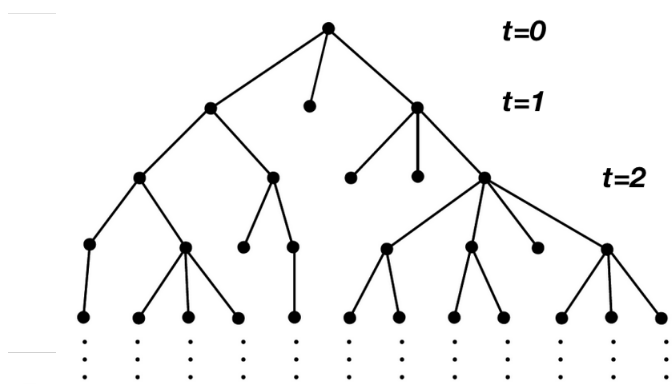

FIG. 1 – *An example of Galton-Watson tree, with $Z_0 = 1$, $Z_1 = 3$, $Z_2 = 5$, etc.*

The number of elements in the $t+1$th generation is obtained from the number of the previous generation t as

$$Z_{t+1} = \sum_{i=1}^{Z_t} K_i \ . \tag{8}$$

K_i is the number of offsprings of the ith element in the t generation. This equation can be used to generate the process, once the probability law $P(K)$ has been chosen.

The question asked by Galton and Watson was *what is the probability of extinction*? Extinction is achieved when $Z_t = 0$, for the first "time". Once $Z_t = 0$, clearly, $Z_{t'>t} = 0$

as well. Extinction is an "absorbing state" of the process. In mathematical terms, the probability of extinction is given by

$$P_{\text{ext}} = \lim_{t\to\infty} P(Z_1 = 0 \ \text{ or } \ Z_2 = 0 \ \text{ or } \ \dots \ \text{ or } \ Z_t = 0) = \lim_{t\to\infty} P(Z_t = 0) \ . \tag{9}$$

We need to find an expression for $P(Z_t = 0)$ and study its long t properties.

We will start by recalling some properties of the generating function of the random variable K (see Math Support)

$$f_K(x) = \sum_{k=0}^{\infty} p_k x^k = \langle x^K \rangle \ . \tag{10}$$

1. Give the values of $f_K(0)$ and $f_K(1)$.
2. Call $m \equiv \langle K \rangle$ and express it in terms of f_K. can you foresee some special value of m which could make change the behaviour of the process in its long time limit?
3. What are the signs of $f'_K(x)$ and $f''_K(x)$?
4. Make a sketch of $f_K(x)$ for $x \in [0{,}1]$.

Let us now define the sum of random variables

$$S = \sum_{i=1}^{N} K_i \tag{11}$$

with N fixed.

5. Show that the generating function of S, $f_S(x)$, is given by $f_S(x) = (f_K(x))^N$, using the fact that the K_i are *i.i.d.*

Imagine now that N is also a random variable, independent from the K ones, and with a different probability distribution.

6. Show that the generating function of S, $f_S(x)$, is now given by $f_S(x) = f_N(f_K(x))$.

We now apply these definitions to the Galton-Watson process.

7. Rewrite f_S, making the corresponding association of variables. Express it as a recursion relation to prove

$$f_{Z_t}(x) = \underbrace{f_K(f_K(f_K(\dots f_K(x))))}_{t-\text{times}} = \underbrace{f_K \circ f_K \circ f_K \circ \dots \circ f_K}_{t-\text{times}}(x) \equiv f_K^{(t)}(x) \tag{12}$$

   where the super-script $^{(t)}$ indicates composition t times (and not power). Give also the initial values of the recursion.
8. Find $\langle Z_t \rangle$ as a function of $m = \langle K \rangle$ and t. Distinguish two relevant cases depending on the value of m.
9. Express now the probability of extinction P_{ext} in eq. (9) in terms of f_K.
10. Solve the iteration that you have just found for P_{ext} graphically, distinguishing two relevant possibilities.
11. In which case is extinction unavoidable? What happens in the other cases? Have you found a sharp change at a particular value of a control parameter? Which is this control parameter?

We have solved the problem in the limit of infinite number of generations, $t \to \infty$. We now consider it for *finite* t, and to make the connection with the *finite size scaling* theory very clear, we call it $t_{\max} = L$. The probability of extinction is simply $P_{\text{ext}}(L) = P(Z_L = 0) = f_K^L(0)$.

12. Is $P_{\text{ext}}(L)$ smaller or larger than $P_{\text{ext}}(t \to \infty)$? Why?
13. Write a code to compute $P_{\text{surv}}(L) = 1 - P_{\text{ext}}(L)$, the survival probability, for the choice $P(K = k) = p(1-p)^k$. Plot $P_{\text{surv}}(L)$ for several values of L (if possible, logarithmically spaced). What do you observe?
14. Try to scale the data for $\sigma_c^2 L P_{\text{surv}}(L)$ using $L(\langle K \rangle - 1)$ as a scaling variable with $\sigma_c^2 = \langle K^2 \rangle - \langle K \rangle^2$. Does it work?
15. Choose another probability distribution for $P(K = k)$, and repeat the procedure. Do you find data collapse on the same scaling function?
16. If we interpret $\sigma_c^2 L P_{\text{surv}}(L)$ as an order parameter, what does the scaling with $L(\langle K \rangle - 1)$ implies for the exponents β and ν?

Références

[1] H. W. Watson and F. Galton, *On the probability of the extinction of families*, J. Anthropol. Inst. Great Britain Ireland, **4**, 138 (1875).

[2] T. E. Harris, *The Theory of Branching Processes* (Springer, Berlin, 1963).

[3] A. Corral and F. Font-Clos, *Criticality and self-organization in branching processes: application to natural hazards*, in *Self-Organized Criticality Systems*, ed. by M. J. Aschwanden (Open Academic Press, Berlin, 2013).

[4] R. García-Millán, F. Font-Clos, and A. Corral, *Finite-size scaling of survival probability in branching processes*, Phys. Rev. E **91**, 042122 (2015).