Mid-term Exam: Statistical Mechanics 2017/18, ICFP Master (first year)

Werner Krauth, Olga Petrova, Jacopo De Nardis
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Introduction

I. METHOD OF MOMENTS AND MAXIMUM LIKELIHOOD

Consider n independent samples $X_1, \dots, X_n$ drawn from a uniform distribution with bounds a and b, where a and b are unknown parameters and $a < b$.

$$X_1, \dots, X_n \sim \text{Uniform}(a, b) \tag{1}$$

1. Explain what a method-of-moments estimator is. For n samples $X_1, \dots, X_n$ and a probability distribution π depending on k parameters $(\theta_1, \dots, \theta_k)$, the method-of-moments estimator is the value $\hat{\theta}$ such that the k lowest moments $\alpha_j = \int x^j \pi(x, \theta) dx$ agree with the sample moments $\hat{\alpha_j} = \sum_{i=1}^n X_i^j$. This is a system of k equations with k unknowns. The method of moments is not optimal, and sometimes the moments of the distribution do not exist, although the sample moments always exist. But the method of moments is easy to use.

2. Find the method-of-moments estimator for a and b. We need to solve

$$\frac{1}{b-a} \int_a^b x dx = \hat{\alpha}_1 \qquad \frac{1}{b-a} \int_a^b x^2 dx = \hat{\alpha}_2 \tag{2}$$

   Therefore we have $(a+b)/2 = \hat{\alpha_1}$ and $\frac{1}{3}(b^3 - a^3)/(b-a) = \frac{1}{3}(a^2 + ab + b^2) = \hat{\alpha_2}$, one finds $b = \hat{\alpha_1} + \sqrt{3}\sqrt{\hat{\alpha_2} - \hat{\alpha_1}^2}$ and $a = \hat{\alpha_1} - \sqrt{3}\sqrt{\hat{\alpha_2} - \hat{\alpha_1}^2}$.

3. Explain the essence of maximum-likelihood estimation, and discuss the difference between a likelihood and a probability. Using the same definitions as above, the likelihood function is defined as the product over the probabilities $\mathcal{G}(\theta) = \prod_{i=1}^n \pi(X_i, \theta)$, and the maximum likelihood estimator is the value of the parameters θ that maximizes this value, as a function of the data.

4. Find the maximum-likelihood estimator $\hat{a}$ and $\hat{b}$. Because of the normalization $(b-a)$, the maximum likelihood estimator is largest if the interval $(b-a)$ is smallest. Therefore, $b = \max(X_i)$ and $a = \min(X_i)$.

II. SPINS IN AN ALTERNATING MAGNETIC FIELD

Consider N spins in an alternating magnetic field

$$H = \mu h \sum_{i=1}^{N} (1 + 2(-1)^i) s_i \tag{3}$$

with $s_i = \pm$. Note that there are no interactions between different spins.

1. What is the partition function of this system?

   Remember that the sum over spins of a factorized function of the spins is the product of each sum, i.e. for any function f we have

$$\sum_{s_1} \sum_{s_2} \cdots \sum_{s_N} \left[\prod_{j=1}^{N} f(s_j) \right] = \prod_{j=1}^{N} \left(\sum_{s_j} f(s_j) \right) \tag{4}$$

   The partition function can then be written by separating odd and even sites as

$$Z = \left(\sum_{s_i = \pm} e^{-3\beta\mu h s_i} \right)^{N/2} \left(\sum_{s_i = \pm} e^{\beta\mu h s_i} \right)^{N/2} = (4\cosh(3\beta\mu h)\cosh(\beta\mu h))^{N/2} \tag{5}$$

2. Find the free energy of this system at temperature T. Then

$$F = -\frac{N}{2}\beta^{-1}\left(\log\left(2\cosh 3\beta\mu h\right) + \log\left(2\cosh\beta\mu h\right)\right) \tag{6}$$

3. What is the magnetization of each spin? Magnetization on is given on even sites by

$$\langle s_i \rangle = \frac{\left(\sum_{s_i=\pm} s e^{-3\beta\mu h s_i}\right)}{\left(\sum_{s_i=\pm} e^{-3\beta\mu H s_i}\right)} = \tanh(3\beta\mu h) \tag{7}$$

and on odd sites by

$$\langle s_i \rangle = \frac{\left(\sum_{s_i=\pm} s e^{\beta\mu h s_i}\right)}{\left(\sum_{s_i=\pm} e^{\beta\mu H s_i}\right)} = -\tanh(\beta\mu h) \tag{8}$$

4. Does this model have a phase transition? No, the model is in 1D and its transfer matrix is finite dimensional and does not contain any zeroes.

III. THE 3-STATE POTTS MODEL IN 1D

The Potts model is a generalization of the Ising model. Rather than having only two possible values as in the Ising case, spins in the Potts model take one of p values (that we take to be $1, \ldots, p$). We consider the case where $p = 3$. The three-state Potts model for a 1D chain of N spins with periodic boundary conditions has the following Hamiltonian:

$$H^{\mathrm{PBC}} = -J \sum_{i=1}^{N} \delta_{s_i, s_{i+1}}, \tag{9}$$

where $\delta_{s_i,s_{i+1}}$ is the Kronecker delta: it is equal to 1 when $s_i = s_{i+1}$ and zero otherwise, and the spin s_{N+1} is the same as s_1.

1. Write down the transfer matrix for this model.

$$T = \begin{bmatrix} e^J & 1 & 1 \\ 1 & e^J & 1 \\ 1 & 1 & e^J \end{bmatrix}$$

where β has been incorporated into $J(T)$.

2. Express the partition function for finite N in terms of the transfer matrix (+ explanation).

$$Z = \sum_{\{s_i\}} e^{J\sum_{i=1}^{N}\delta_{s_i,s_{i+1}}} = Tr[T^N] \tag{10}$$

3. How would you go about computing the partition function in the limit $N \to \infty$? (Don't do the calculation, just explain how it is done and why).

$$Z = \lambda_0^N + \lambda_1^N + \lambda_2^N$$

where λ_i are the three eigenvalues of T. In the limit $N \to \infty$, it suffices to keep the largest eigenvalue λ_0:

$$Z \approx \lambda_0^N$$

.

4. Consider now the case of open boundary conditions, with the hamiltonian given by

$$H^{\text{open}} = -J \sum_{i=1}^{N-1} \delta_{s_i, s_{i+1}}. \tag{11}$$

(a) Express the partition function of the Potts model of N spins in terms of the transfer matrix for the case of special boundary conditions $s_1 = 1$, $s_N = 1$.

$$Z = \vec{A}^t T^{N-1} \vec{A} \tag{12}$$

with

$$\vec{A}^t = (1, 0, 0) \tag{13}$$

in other words, the $(1,1)$ element of the transfer matrix taken to the power $N-1$. For $N = 2$, this is easy to check as there is only one configuration, so that $Z_2 = \exp(J)$. Note that there are only $N-1$ terms in the hamiltonian of eq. (**??**).

(b) Express the partition function of the Potts model of N spins in terms of the transfer matrix for the case of open boundary conditions, where both s_1 and s_N can take on all three values.

$$Z = \vec{A}^t T^{N-1} \vec{A} \tag{14}$$

with

$$\vec{A}^t = (1, 1, 1) \tag{15}$$

in other words, the sum over all the elements of the transfer matrix taken to the power $N-1$. For $N = 2$, this is easy to check as there are 9 configuration, three of them with weight $\exp(J)$ and six of them with weight 1. This agrees with the sum over all the terms of $T = T^{N-1}$ for $N = 2$.

IV. CLUSTER EXPANSION FOR AN INTERACTING GAS

Consider a gas of N particles in a one-dimensional box of size L (with density $N/L = \rho$ fixed) with Hamiltonian

$$H = \sum_{i=1}^{N} p_i^2 + \sum_{i<j,=1}^{N} U(q_i - q_j) \tag{16}$$

with the interparticle potential given by

$$U(q) = 0 \text{ if } q > a \tag{17}$$

$$U(q) = u_0 \text{ if } q \le a \tag{18}$$

We want to compute the free energy as an expansion in u_0 up to orders u_0^2 (we neglect terms of order u_0^n with $n > 2$). Consider the partition function

$$Z = \left(\prod_{j=1}^{N} \int_0^L dq_j \int_{-\infty}^{+\infty} dp_j \right) \prod_{i=1}^{N} e^{-\beta p_i^2} \prod_{i<j} e^{-\beta U(q_i - q_j)} = Z_0 Q \tag{19}$$

with

$$Q = L^{-N} \left(\prod_{j=1}^{N} \int_0^L dq_j \right) \prod_{i<j} e^{-\beta U(q_i - q_j)} \tag{20}$$

and Z_0 the partition function of the free gas (with $u_0 = 0$). Write the free energy of the non-interacting gas as $F_0 = -\beta^{-1} \log Z_0$.

1. Write down the partition function of the free Gas $F_0 = -\beta^{-1} \log Z_0$

$$F_0 = -\beta^{-1} N \log\left(L \int dp e^{-\beta p^2}\right) = -\beta^{-1} N \log(\sqrt{\pi/\beta} L) \tag{21}$$

2. Expand Q up to the order u_0^2 and compute the free energy $F = -\beta^{-1} \log Z_0 - \beta^{-1} \log Q$. You should find

$$F = F_0 - \beta^{-1} N \,(\text{corrections }) \tag{22}$$

with the corrections depending on β, ρ, a and clearly u_0 and u_0^2.
In order to expand Q write $e^{-\beta U(q_i - q_j)} = 1 + f_{i,j}$, then we have

$$Q = 1 + \sum_{i<j} L^{-2} \int dq_i dq_j \left(e^{-\beta U(q_i-q_j)} - 1\right) + \sum_{i<j} \sum_{k<l} L^{-4} \int dq_i dq_j dq_k dq_l \left(e^{-\beta U(q_k-q_l)} - 1\right)\left(e^{-\beta U(q_i-q_j)} - 1\right) + \dots \tag{23}$$

In the first term expand $\left(e^{-\beta U(q_i-q_j)} - 1\right) = -\beta u_0 + \frac{(\beta u_0)^2}{2}$ when $q_j \in [q_i - a, q_i + a]$. Then the first term gives

$$\sum_{i<j} L^{-2} \int_0^L dq_i \int_{q_i-a}^{q_i+a} dq_j \left(e^{-\beta U(q_i-q_j)} - 1\right) = \frac{N-1}{2}\frac{N}{L}(2a)\left(-\beta u_0 + \frac{(\beta u_0)^2}{2}\right) \tag{24}$$

For the second term we need to distinguish between the cases where $j = k$ and where $j \neq k$. The first cases produces

$$\sum_{i<j<l} L^{-3} \int dq_i dq_j dq_l \left(e^{-\beta U(q_i-q_j)} - 1\right)\left(e^{-\beta U(q_j-q_l)} - 1\right) = \frac{N}{3!}\left(\frac{N}{L}\right)^2 (2a\beta u_0)^2 + O(1/N) \tag{25}$$

where we used that $\sum_{i<j<l} = N(N-1)(N-2)/3! \sim N^3/3!$. The other contributions with $j \neq k$ produce disconnected diagrams (whose number grows with N^4). Remember that disconnected diagram do not contribute when we take the log of Z (linked cluster theorem). Therefore we can write the Free energy as

$$F = F_0 - \beta^{-1} \log\left[1 + N\left(\frac{(2a\rho)}{2}\left(-\beta u_0 + \frac{(\beta u_0)^2}{2}\right) + \rho^2 \frac{(2a\beta u_0)^2}{6} + O(u_0^3)\right)\right] \tag{26}$$

Expanding the log as $\log(1 + x) = x + \dots$

$$F = F_0 - \beta^{-1} N\left[\left(\frac{(2a\rho)}{2}\left(-\beta u_0 + \frac{(\beta u_0)^2}{2}\right) + \rho^2 \frac{(2a\beta u_0)^2}{6} + O(u_0^3)\right)\right] \tag{27}$$

Notice that disconnected diagram would have contributed with corrections of order N^2 to the free energy, which is indeed not physical (free energy has to be an extensive function of N).