Calculating normalizing factors: a short review

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1 Introduction

Calculating normalizing factors with Monte Carlo (MC) simulations is a fundamental problem throughout many scientific and statistical scenarios. In statistical physics, the logarithmic of the normalizing factor of a given Gibbs distribution relates to the Helmholz free energy and thermodynamic entropy, which comprises the information of phase transition.

Historically, the phenomenon of coexistence of a first-order transition poses great challenge to direct MC simulations as it generates a large free energy barrier to separate the two phases. To approach this problem, some more robust methods are prefered. This note reviews some of those methods by starting with the method of *thermodynamic integration (TI)*, which, in addition to the applications on obtaining the free energy, can be used to calculate more general normalizing factors.

The idea of TI can date back to late 1970's, as pointed out by Y. Ogata [1], a statistician, who independently proposed the idea of TI to provide a solution to the objective Bayesian method [2] without the awareness of the progress in statistical physics at the beginning. To learn the progress of TI and other related methods in classical MC before 2000, I suggest readers follow Ref. [3, 4], which together with Ref. [5], a systematic introduction of TI, are main references of this note.

2 Thermodynamic integration

Suppose we have two systems A and B with potential energies E_A and E_B, respectively, then the basic idea of this method is to compute the *free energy difference* or the *partition function difference* between A and B from some integration process.

We first assume that A and B share the same temperature T. In general, we can consider an integration from A to B by defining an extended system, which has the potential energy $E(\lambda)$ as the function of

E_A, E_B and $\lambda \in [0,1]$. It satisfy that $E(0) = E_A$ and $E(1) = E_B$. One possible form of such a function is

$$E(\lambda) = E_A + \lambda(E_B - E_A) \tag{1}$$

but remember that $E(\lambda)$ can be more general theoretically.

In the canonical ensemble, the partition function (normalizing factor) is

$$Z(\lambda) = \sum_c e^{-E_c(\lambda)/T} \tag{2}$$

where the Boltzmann constant k_B is set to be unit. Therefore, we have

$$\begin{aligned} \frac{d\ln Z(\lambda)}{d\lambda} =& \frac{1}{Z(\lambda)} \frac{dZ(\lambda)}{d\lambda} \\ =& -\frac{1}{T}\frac{1}{Z(\lambda)} \sum_c e^{-E_c(\lambda)/T} \frac{dE_c(\lambda)}{d\lambda} \\ =& -\frac{1}{T}\left\langle \frac{dE_c(\lambda)}{d\lambda} \right\rangle_\lambda \end{aligned} \tag{3}$$

Similarly, we can also discuss the case that A and B differ in temperature. For convenience, we consider the inverse temperature $\beta = 1/T$, then with some algebra, we can derive

$$\frac{d\ln Z(\beta)}{d\beta} = -\langle E_c(\beta)\rangle_\beta \tag{4}$$

Notice that A and B also do not need to be exactly the same system, and $E(\beta)$ can be some artifically defined extended function such as $E(\beta) = E_A + \beta(E_B - E_A)$.

Integrating Eq. (3) and Eq. (4), we can obtain the (logarithmic) partition function difference as

$$\ln \frac{Z_B}{Z_A} = \int_0^1 -\frac{1}{T}\left\langle dE_c(\lambda) \right\rangle_\lambda \tag{5}$$

and

$$\ln \frac{Z_B}{Z_A} = \int_{\beta_A}^{\beta_B} -\left\langle E(\beta) \right\rangle_\beta d\beta \tag{6}$$

The way that obatining the partition function or free energy using Eq. (5) or Eq. (6) is called TI.

An important comment is that since we are considering the partition function/normalizing factor difference between A and B, the initial set-up can be based on Z_A and Z_B directly, rather than from E_A and E_B.

Fir numerical considerations, taking Eq. (5) as an example, we should calculate the summation

$$\ln \frac{Z_B}{Z_A} = \sum_{i=0}^{m} -\frac{1}{T}\Big[E(\lambda_{i+1}) - E(\lambda_i)\Big] \tag{7}$$

Eq. (7) requires a bulk of intermidiate steps to reduce the numerical integral errors, yet it is general and powerful.

Akin to *simulated annealing* method, one can prepare the initial state at λ_{i+1} with the final state at λ_i from previous simulations, but one have to take care of the local minimum problem. For example, if we integrate by temperature, we should start from a high temperature and decrease it. Each sample we obtain in this sense is actually a path in the phase space spanned by both the degree of configurations and λ. It enables us to apply the *Jarzynski equality* to achieve the final result [6]. One representative variant of TI recently is calculating the entanglement entropy, which is also a generalized normalizing factor, via non-equilibrium work [7].

3 Simple importance sampling

A variant of TI is a direct evaluation of $\ln(Z_B/Z_A)$ by simple sampling, which is also called TI in many literatures [8, 9].

Suppose $Z_A = \sum_c W_c^A$ and $Z_B = \sum_c W_c^B$ in some extended configuration space $\{c\}$, then

$$\frac{Z_B}{Z_A} = \left\langle \frac{W_c^B}{W_c^A} \right\rangle_A \tag{8}$$

Eq. (8) is also known as the *reweighting* technique in MC simulations. The extended configuration space is to ensure the overlap between two distributions Z_A and Z_B can be well defined. A trivial example is that $Z_A = W_{s_1}$ and $Z_B = W_{s_2}$, then by defining the extended space $\{c_1 \equiv s_1, c_2 \equiv s_2\}$, we can write $Z_A = W_{c_1} + W_{c_2}$ with $W_{c_2} = 0$.

Because of the existence of zero weight, this trival example obviously cannot be calculated via Eq. (8). At least, the configuration space of A should encompass that of B. Therefore, the extended configurations space indicates the requirement of a great overlap between Z_A and Z_B to make the evaluation of Eq. (8) efficient. In other words, the importance sampling is needed.

To ensure the importance sampling, some intermidiate systems are often introduced. It is also called multi-statge sampling, bridge sampling, or just interpolation in some literatures [10, 3]. Specifically, we consider

$$\frac{Z_B}{Z_A} = \frac{Z_B}{Z_{a_1}} \frac{Z_{a_2}}{Z_{a_3}} \cdots \frac{Z_{a_{m-1}}}{Z_A} \tag{9}$$

The choice of $\{Z_{a_i}\}$ represents a specific path, on which each intermidiate process $Z_{a_i}/Z_{a_{i+1}}$ satisfies the condition of importance sampling. Similarly, rather than estimating each $Z_{a_i}/Z_{a_{i+1}}$ independently, we can take the same trick as that introduced in the last paragraph in the last section. For this application, equilibrium must be satisfied.

There have been many interesting variants of this method, and I review some of them here.

3.1 Different boundary conditions

K. K. Mon (1985) considered Z_A and Z_B to be a same model but with totally different bounary condistions [10]. For the 2D Ising model: Z_A is for a $2N \times 2N$ lattice with a standard perodic boundary condition (PBC); Z_B is a composite system of four $N \times N$ lattices, each of them has the PBC. The intermidiate stages defined in this work is effectively $H(\lambda) = \lambda H_A + (1-\lambda)H_B$.

3.2 Estimating expectation values and the "snake" algorithm

One more step forward, we can set $Z_A = \mathrm{Tr}(\rho)$ to be some standard partition function, and $Z_B = \mathrm{Tr}(\rho O)$ to denote the unnormalized expectation value of some operator O. Thus

$$\frac{Z_B}{Z_A} = \frac{\mathrm{Tr}(\rho O)}{\mathrm{Tr}(\rho)} \tag{10}$$

denotes the expectation value.

One representive example is the *"snake" algorithm* proposed by P. de Forcrand, M. D'Elia, and M. Pepe, in 2001, in which they considered the 't Hooft loop expectation value in SU(2) Yang-Mills lattice gauge theory (LGT) [11]. I have no idea why they called this "snake" algorithm, but the idea is straightforward.

In their set-up, Z_B represents partition function including all the loop excitations, and Z_A is the vanilla partition function with no loop excitations. Then they considered

$$\frac{Z_B}{Z_A} = \frac{Z_N}{Z_0} = \frac{Z_N}{Z_{N-1}}\frac{Z_{N-1}}{Z_{N-2}}\cdots\frac{Z_1}{Z_0} \tag{11}$$

where Z_i denotes the intermidiate stages with i loop excitations or flipped plaquettes.

The applications of the "snake" algorithm on LGTs can also be found in Ref. [12, 13]

The key idea of this variant of TI is to find a good series of intermidiate stages based on the problem we consider. Another example, by M. Caselle, M. Hasenbusch, and M. Panero (2003), was to calculating the Green's function

$$G(R) = \langle P(x)P^\dagger(x+R)\rangle \tag{12}$$

where $P(x)$ loop operator at position x in the confined phase of a LGT. They considered a quantity defined as $Q(R) = \ln[G(R)/G(R+1)]$ to cancel the normalizing factor. The intermidiate stages are chosen to gradually put some spins inside the full manifold. More details can be found in [14], which is similar to that in [7], but the latter one did not consider the ratio form of TI. One more similar example suggested is by M. Hasenbusch (2009), where he used similar technique to calculate the Casimir force [15].

4 Bennett accpetance ratio method

Recall that for Eq. (8), if A can be in some state that B cannot, and vice versa, then we should exquisitely design the intermidiate stages to ensure importance sampling. Another way to fix this is to sample in the extended configuration space, and this is called the *(Bennett) accpetance ratio method*, and the earliest work of it is given in Ref. [16] by C. H. Bennett in 1976. In this language, Z_B/Z_A is interpreted as the ratio of the fractions of two subregions B and A in the extended system.

Let us clarify some notations to introduce the method. For two systems A and B with internal energy E_A and E_B, we define the energy function E_* of the extended system to be

$$E_*(c,w) = \begin{cases} E_A(c)/T_A & \text{if } w = 0 \\ E_B(c)/T_B & \text{if } w = 1 \end{cases} \tag{13}$$

where c denotes the configuration in A or B. The temperature of this extended system is thus one. The extended configuration space is now $\{(c,w)\}$, so the update of the configuration should include w.

The conditional distributions in this case are

$$\begin{aligned} p(w=0|c) &= \frac{e^{-E_*(c,0)}}{e^{-E_*(c,0)} + e^{-E_*(c,1)}} \\ p(w=1|c) &= \frac{e^{-E_*(c,1)}}{e^{-E_*(c,0)} + e^{-E_*(c,1)}} \end{aligned} \tag{14}$$

The transfer between $(c,0)$ to $(c,1)$ can be designed based on the standard Metroplis-Hasting algorithm, and marginally

$$\frac{\int \frac{1}{Z_*} e^{-E_B(c)/T_B} dc}{\int \frac{1}{Z_*} e^{-E_A(c)/T_A} dc} = \frac{p(w=1)}{p(w=0)} = \frac{Z_B}{Z_A} \tag{15}$$

Eq. (13) is not the only and best choice to define such an extended system and implement the acceptance ratio method. For more detailed introduction and discussions, please refer to Ref. [17].

5 More methods

5.1 Umbrella sampling

If A and B are separated by huge energy barrier, then it is hard to go over the full energy landscape to give an accurate estimation of the free energy difference. The *umbrella sampling*, proposed by G.M. Torrie and J.P. Valleau in 1977, is a method aiming to bridge the gap [18].

For the estimation of Z_B/Z_A with Eq. (8), rather than sample on the system A, we introduce a biased and auxiliary system, denoted as D, whose distribution is given by

$$p_D(c) = \frac{1}{Z_D}\tilde{\omega}\left[\frac{W_c^B}{W_c^A}\right]e^{-E_A(c)/T_A} \tag{16}$$

where $\tilde{\omega}$ is a biased function, usually given by trials for a better estimation of W_c^B/W_c^A. Then Eq. (8) can be rewritten as

$$\frac{Z_B}{Z_A} = \langle O_{AB}\rangle_A = \frac{\langle O_{AB}/\tilde{\omega}\rangle_D}{\langle 1/\tilde{\omega}\rangle_D} \tag{17}$$

where $O_{AB} := W_c^B/W_c^A$, which is similar to the way we consider the sign problem in quantum Monte Carlo. About more details of umbrella sampling as well as the choice of $\tilde{\omega}$ can be found in Ref. [19].

5.2 Wang-Landau sampling

To be edited...

F. Wang, and D.P. Landau (2001). [20].

5.3 Escorted free-energy perturbation

To be edited...

C. Jarzynski (2002); S. Vaikuntanathan and C. Jarzynski (2008) [21, 22].

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