Overview of the reweighting trick

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1 Introduction

Consider a partition function $Z(\beta) = \sum_C e^{-\beta E(C)}$ at the (inverse) temperature point β, and some observable $\mathscr{O}$, then

$$\langle \mathscr{O} \rangle_\beta = \sum_C p(\beta, C)\mathscr{O}(C) = \sum_C \frac{e^{-\beta E(C)}}{Z(\beta)}\mathscr{O}(C) \tag{1}$$

which can be estimated via Monte Carlo (MC) simulations and the subscript β denotes that the sampling is performed at temperature β.

The question here is **what if we can only simulate at β'? Can we obtain the estimation of $\langle \mathscr{O} \rangle_\beta$ as well**? The answer is yes, and this is where we resort to the protagonist of this note, the *reweighting*.

The concept of reweighting was first proposed in [M. Karplus, J. Chem. Phys. 30, 11–15 (1959)], and an early representative application can be found in [A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. 61, 2635 (1988)]. It is an important and useful technique used in many algorithms like some multihistogram method [A. M. Ferrenberg and R. H. Swendsen, Phys. Rev. Lett. 63, 1195 (1989)], and the reweight-annealing MC framework for calculating partition functions [Y.M. Ding *et al.* arXiv:2403.08642], [Z. Wang *et al.* arXiv:2406.05324].

In Sec. 2, we will introduce the concept of reweighting with the example of classical MC and the temperature case. It is straightforward to generalize the discussions to quantum Monte Carlo and other parameters such as some coupling strength in the Hamiltonian. In Sec. 3, we will discuss the mathematical relation between reweighting and the moment-generating function (MGF).

2 Reweighting

We first rewrite the probability $p(\beta, C)$ with $Z(\beta')$ in Eq. (1), which is

$$p(\beta, C) = \frac{e^{-\beta E(C)}}{Z(\beta)} = \frac{Z(\beta')}{Z(\beta)} e^{-(\beta-\beta')E(C)} \frac{e^{-\beta' E(C)}}{Z(\beta')} \tag{2}$$

then

$$\begin{aligned}\langle\mathscr{O}\rangle_\beta =&\sum_C p(\beta,C)\mathscr{O}(C)\\ =&\frac{Z(\beta')}{Z(\beta)}\sum_C e^{-(\beta-\beta')E(C)}\frac{e^{-\beta' E(C)}}{Z(\beta')}\mathscr{O}(C)\\ =&\frac{Z(\beta')}{Z(\beta)}\langle\mathscr{O}e^{-(\beta-\beta')E}\rangle_{\beta'}\end{aligned}\tag{3}$$

The ratio $Z(\beta')/Z(\beta)$ in Eq. (3) can be achieved by substituting $\mathscr{O}=1$, which leads to

$$\frac{Z(\beta)}{Z(\beta')}=\langle e^{-(\beta-\beta')E}\rangle_{\beta'}\tag{4}$$

then

$$\langle\mathscr{O}\rangle_\beta=\frac{\langle\mathscr{O}e^{-(\beta-\beta')E}\rangle_{\beta'}}{\langle e^{-(\beta-\beta')E}\rangle_{\beta'}}\tag{5}$$

Finally, we successfully transfer our estimation of $\langle\mathscr{O}(\beta)\rangle_\beta$ at β to some estimations at temperature β'. Using Eq. (5), we can (in principle) obtain the information of the system at any other temperature β only by sampling at a fixed temperature point β'.

Notice that the factor $e^{-(\beta-\beta')E}$ occurs in both Eq. (4) and (5). This is actually the average weight ratio of the weights in $Z(\beta)$ and $Z(\beta')$ for a same configuration. By extracting this factor, we effectively rearrange the weight of each configuration, and this is why we call the trick reweighting.

3 Reweighting and MGF

The partition function ratio in Eq. (4) is actually a special case of a MGF, which is defined as

$$M_X(\tau)=\mathbb{E}(e^{\tau X})=1+\tau\mathbb{E}(X)+\frac{\tau^2}{2!}\mathbb{E}(X^2)+\cdots+\frac{\tau^n}{n!}\mathbb{E}(X^n)+\cdots\tag{6}$$

where X is some random variable and τ is a real number. If we take X to be the energy $E\in\{E(C)\}$ at temperature β', then the MGF is written as

$$M_E(\tau)=\sum_C\frac{e^{-\beta' E(C)}}{Z(\beta')}e^{\tau E(C)}=\frac{1}{Z(\beta')}\sum_C e^{-(\beta'-\tau)E(C)}=\frac{Z(\beta'-\tau)}{Z(\beta')}\tag{7}$$

By identifying $\beta\equiv\beta'-\tau$, we reobtain the ratio in Eq. (4). The MGF intepretation of $Z(\beta)/Z(\beta')$ enables us to utilize its properties to gain the nth moment of E at temperature β', which is

$$\langle E^n\rangle=M_X^{(n)}(0)=\frac{d^n}{d\tau^n}\frac{Z(\beta'-\tau)}{Z(\beta')}\bigg|_{\tau=0}=(-1)^n\frac{Z^{(n)}(\beta')}{Z(\beta')}\tag{8}$$