1 Data reweighting

We consider a generic system with state space S and Hamiltonian H. For simplicity, we assume the configuration space to be discrete (for definiteness imagine the Ising system) but everything can be generalized to continuous configuration spaces. We work in the canonical ensemble, assuming that configurations x are distributed according to the Boltzmann-Gibbs probability density

$$\pi_\beta(x) = \frac{e^{-\beta H(x)}}{Z_\beta} ,$$

where $H(x)$ is the energy function and the normalizing constant Z_β is the partition function at inverse temperature β:

$$Z_\beta = \sum_x e^{-\beta H(x)}.$$

We indicate by $\langle\cdot\rangle_\beta$ the average with respect to $\pi_\beta(x)$.
Here we will address two problems:

1) Suppose we perform a MC simulation at inverse temperature β_0; can we use the same data to compute average values at $\beta_1 \neq \beta_0$?

2) Using again data at β_0, can we compute free energies at different values of β?

As we shall discuss below, the answer to the first question is positive as long as $|\beta_0 - \beta_1|$ is small. The answer to the second question is negative (MC simulations are not able to compute partition functions or, equivalently, free energies); however, the answer is positive if we already know the free energy at β_0 (computed by means of some other method, not by Monte Carlo). The general class of methods that are used in this context are called *reweighting methods*.
If $A(x)$ is any observable, its average at β_1 can be expressed as

$$\begin{aligned}
\langle A\rangle_{\beta_1} &= \frac{\sum_x A(x)e^{-\beta_1 H(x)}}{\sum_x e^{-\beta_1 H(x)}} = \frac{\sum_x A(x)e^{-\beta_0 H(x)}e^{\beta_0 H(x)-\beta_1 H(x)}}{\sum_x e^{-\beta_0 H(x)}e^{\beta_0 H(x)-\beta_1 H(x)}} = \\
&= \frac{\frac{1}{Z_{\beta_0}}\sum_x A(x)e^{-\Delta\beta H(x)}e^{-\beta_0 H(x)}}{\frac{1}{Z_{\beta_0}}\sum_x e^{-\Delta\beta H(x)}e^{-\beta_0 H(x)}} = \frac{\langle A\, e^{-\Delta\beta H}\rangle_{\beta_0}}{\langle e^{-\Delta\beta H}\rangle_{\beta_0}} ,
\end{aligned}$$

where $\Delta\beta = \beta_1 - \beta_0$. To compute the Helmholtz free energy $F(\beta) = -\beta^{-1}\ln Z_\beta$, we write

$$\begin{aligned}
\beta_1 F(\beta_1) &= -\ln\sum_x e^{\beta_1 H(x)} = -\ln\sum_x e^{-\beta_0 H(x)}e^{\beta_0 H(x)-\beta_1 H(x)} = -\ln[Z_{\beta_0}\langle e^{-\Delta\beta H}\rangle_{\beta_0}] \\
&= -\ln Z_{\beta_0} - \ln\langle e^{-\Delta\beta H}\rangle_{\beta_0} = \beta_0 F(\beta_0) - \ln\langle e^{-\Delta\beta H}\rangle_{\beta_0}
\end{aligned}$$

Both calculations involve the same type of averages: they depend on $e^{-\Delta\beta H}$.
Though in principle the previous formulae solve the problem, in practice they are only useful if the averages at β_0 can be computed with reasonable accuracy. But this is not obvious since H is extensive with fluctuations of order $\sqrt{N}$. At β_0, H fluctuates around the mean value E_0 with fluctuations $\pm a\sqrt{N}$ ($a > 0$). Roughly speaking, this implies that $e^{-\Delta\beta H}$ fluctuates between $Me^{-\Delta\beta a\sqrt{N}}$ and $Me^{+\Delta\beta a\sqrt{N}}$, $M = \langle e^{-\Delta\beta H}\rangle_{\beta_0}$. Thus, when computing the sample mean of $e^{-\Delta\beta H}$,

one sums very large and very small numbers: effectively the results is dominated by the few largest numbers obtained in the simulation. Correspondingly, the error is large. Reasonable errors are only obtained if $\Delta\beta$ is so small that $\sqrt{N}\Delta\beta$ is a number of order one. This implies that the method works only in an interval around β_0 that shrinks as N increases.

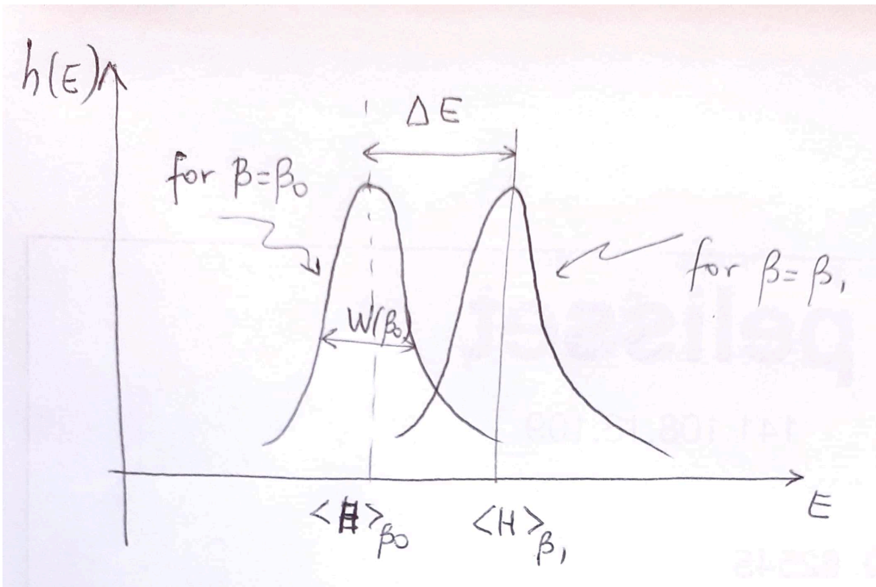

Figure 1: Define $E_1 = \langle H\rangle_{\beta_1}$, $E_0 = \langle H\rangle_{\beta_0}$, $\Delta E = E_1 - E_0$. The width of the distribution can be characterized by the standard deviation $\sigma(E)$. The two distributions overlap if $\Delta E \lesssim \sigma(\beta_0)$ (note that this is a qualitative statement; do not ask yourself the question whether the condition should include some constant, say, be, for instance $\Delta E \lesssim 2\sigma(\beta_0)$, or similar).

This argument can be reformulated, considering the probability $h(E,\beta)$ of configurations of energy E at temperature β. This distribution has a width that can be characterized by the variance

$$\sigma(\beta)^2 = \langle H(x)^2\rangle_\beta - \langle H(x)\rangle_\beta^2 = kT^2 C_v(T) = \hat{C}(T),$$

where

$$C_v(T) = \frac{\partial E}{\partial T}, \qquad \hat{C}(T) = -\frac{\partial E}{\partial \beta}.$$

Now the physical argument is the following. We expect to be able to estimate an average at β_1 only if we explore the configurations that are *typical* at β_1 in the simulation at β_0. This only occurs if the distributions of the typical configurations at β_0 and β_1 overlap. In other words, if E_0 and E_1 are the average values for β_0 and β_1, if $E_1 > E_0$ (this is the case of the figure), we expect the method to work if

$$E_0 + \sigma(\beta_0) \gtrsim E_1 \qquad E_1 - E_0 \lesssim \sigma(\beta_0)$$

If $E_1 < E_0$, we would require $E_0 - E_1 \lesssim \sigma(\beta_0)$, so that the general condition is

$$|E_1 - E_0| \lesssim \sigma(\beta_0)$$

Now, for $\Delta\beta$ small,

$$E_1 - E_0 = E(\beta_1) - E(\beta_0) \approx [E(\beta_0) - \Delta\beta \hat{C}(\beta_0)] - E(\beta_0) \approx -\Delta\beta\, \hat{C}(\beta_0)$$

The condition becomes

$$|\Delta\beta| \hat{C}(\beta_0) \lesssim \sqrt{\hat{C}(\beta_0)} \qquad |\Delta\beta| \lesssim \frac{1}{\sqrt{\hat{C}(\beta_0)}}$$

Now, note the $\hat{C}(\beta_0)$ is extensive (proportional to N), and therefore we obtain

$$|\Delta\beta| \lesssim \frac{b}{\sqrt{N}}.$$

This is a general property of all reweighting methods: the temperature interval in which the procedure works shrinks as $1/\sqrt{N}$ as N increases.

We wish now to make this qualitative discussion more quantitative. For this purpose, let us compute the statistical error on $\langle A \rangle_{\beta_1}$. Since this quantity is expressed as a ratio of two mean values, the variance of the estimator (remember, variance with respect to MC repetitions, in equilibrium) can be obtained by using the general expression

$$\sigma^2_{\text{est}} \equiv \text{var}\left(\frac{\frac{1}{n}\sum_i A_i}{\frac{1}{n}\sum_i B_i} \right) = \frac{1}{n} \frac{\langle A \rangle^2}{\langle B \rangle^2} \left\langle \mathcal{O}^2 \right\rangle 2\tau_{\mathcal{O}} + O(n^{-2}) \;, \tag{1}$$

where n is the number of measurements performed,

$$\mathcal{O} = \frac{A}{\langle A \rangle} - \frac{B}{\langle B \rangle} \;, \tag{2}$$

and $\tau_{\mathcal{O}}$ is the integrated autocorrelation time associated with $\mathcal{O}$. Eq. (1) is valid as $n \to \infty$, neglecting corrections of order n^{-2}. In our case the relevant quantity is $\left\langle \mathcal{O}^2 \right\rangle$. If we specialize Eq. (2) to our case, we obtain

$$\langle \mathcal{O}^2 \rangle_0 = \left\langle \left(\frac{A e^{-\Delta\beta H}}{\langle A e^{-\Delta\beta H} \rangle_0} - \frac{e^{-\Delta\beta H}}{\langle e^{-\Delta\beta H} \rangle_0} \right)^2 \right\rangle_0$$

where $\langle \cdot \rangle_{\beta_0} = \langle \cdot \rangle_0$. Now, if $A_1 = \langle A \rangle_{\beta_1}$ we have

$$\langle A e^{-\Delta\beta H} \rangle_0 = A_1 \langle e^{-\Delta\beta H} \rangle_0$$

Substituting, we get

$$\langle \mathcal{O}^2 \rangle_0 = \left\langle \left(\frac{A}{A_1} - 1 \right)^2 \frac{e^{-2\Delta\beta H}}{\langle e^{-\Delta\beta H} \rangle_0^2} \right\rangle_0$$

Now, we define $\beta_2 = 2\beta_1 - \beta_0$. Since

$$\beta_1 = \frac{\beta_0 + \beta_2}{2}$$

it is easy to understand what β_2 is: it is the symmetric point of β_0 with respect to β_1 (β_1 is the midpoint of the segment connecting β_0 and β_2 on the β-line). It follows $\beta_2 - \beta_1 = \beta_1 - \beta_0 = \Delta\beta$ and $\beta_2 - \beta_0 = 2(\beta_1 - \beta_0) = 2\Delta\beta$, which implies

$$\langle B \rangle_2 = \frac{\langle B e^{-(\beta_2 - \beta_0)H} \rangle_0}{\langle e^{-(\beta_2 - \beta_0)H} \rangle_0} = \frac{\langle B e^{-2\Delta\beta H} \rangle_0}{\langle e^{-2\Delta\beta H} \rangle_0}.$$

We can thus rewrite

$$\langle \mathcal{O}^2 \rangle_0 = \left\langle \left(\frac{A}{A_1} - 1 \right)^2 \right\rangle_2 \frac{\left\langle e^{-2\Delta\beta H} \right\rangle_0}{\langle e^{-\Delta\beta H} \rangle_0^2}$$

Finally, in terms of the Helmholtz free energy $F(\beta)$ we have

$$\left\langle e^{-2\Delta\beta H} \right\rangle_0 = \exp[\beta_0 F(\beta_0) - \beta_2 F(\beta_2)] \qquad \left\langle e^{-\Delta\beta H} \right\rangle_0 = \exp[\beta_0 F(\beta_0) - \beta_1 F(\beta_1)]$$

We thus obtain the final formula:

$$\langle \mathcal{O}^2 \rangle_0 = \left\langle \left(\frac{A}{A_1} - 1 \right)^2 \right\rangle_2 e^{\mathcal{F}(\beta_0, \beta_1)} ,$$

where

$$\mathcal{F}(\beta_0, \beta_1) = 2\beta_1 F(\beta_1) - \beta_0 F(\beta_0) - \beta_2 F(\beta_2) .$$

Collecting all terms we obtain for the square of the relative error:

$$\frac{\sigma^2_{\text{est}}}{\langle A \rangle_1^2} = \frac{1}{n} \frac{\langle (A - A_1)^2 \rangle_2}{A_1^2} e^{\mathcal{F}(\beta_0, \beta_1)} 2\tau_{\mathcal{O}} + O(n^{-2}) .$$

This result shows that the error on the reweighted result depends on the autocorrelation time (obvious!), and on $\langle (A - A_1)^2 \rangle_2$, which is some kind of variance of the observable and is a slowly varying function of β_1. The relevant term is the exponential term, which is an exponential of an extensive (as we shall prove, positive) quantity. The latter term is the one that controls the error. We wish now to rewrite $\mathcal{F}(\beta_0, \beta_1)$ using $E = \partial(\beta F)/\partial\beta$ and $\hat{C} = -\partial E/\partial\beta$. Now, we have

$$\int_{\beta_0}^{\beta_1} E d\beta = \int_{\beta_0}^{\beta_1} \frac{\partial(\beta F)}{\partial \beta} d\beta = \beta_1 F(\beta_1) - \beta_0 F(\beta_0); \tag{3}$$

Since the same relation holds with β_2 replacing β_0 we have

$$\mathcal{F}(\beta_0, \beta_1) = \int_{\beta_0}^{\beta_1} E d\beta + \int_{\beta_2}^{\beta_1} E d\beta.$$

Now, we rewrite:

$$\int_{\beta_0}^{\beta_1} E d\beta = \int_{\beta_0}^{\beta_1} d\beta E \frac{d}{d\beta}(\beta - \beta_0) = E(\beta_1)(\beta_1 - \beta_0) + \int_{\beta_0}^{\beta_1} d\beta \hat{C}(\beta)(\beta - \beta_0),$$

where we have performed an integration by parts in the last step. The same relation holds for β_2 replacing β_0. Since $\beta_1 - \beta_0 = -(\beta_1 - \beta_2)$ we obtain

$$\mathcal{F}(\beta_0, \beta_1) = \int_{\beta_0}^{\beta_1} d\beta \hat{C}(\beta)(\beta - \beta_0) + \int_{\beta_2}^{\beta_1} d\beta \hat{C}(\beta)(\beta - \beta_2)$$

We now show that both integrals are positive and increasing functions of $|\Delta\beta|$. Assume that $\beta_1 > \beta_0$ so that $\beta_2 > \beta_1$. We can write

$$\mathcal{F}(\beta_0, \beta_1) = \int_{\beta_0}^{\beta_0 + \Delta\beta} d\beta \hat{C}(\beta)(\beta - \beta_0) + \int_{\beta_1}^{\beta_1 + \Delta\beta} d\beta \hat{C}(\beta)(\beta_2 - \beta)$$

In the second integral we have interchanged the endpoints and replaced $\beta - \beta_2$ with $-(\beta_2 - \beta)$. Since the specific heat is always positive, the arguments of the two integrals are both positive. It is also immediate to verify that they increase with $\Delta\beta$ increasing. The same considerations apply $\beta_1 < \beta_0$.

Finally, let us obtain a simpler formula that applies when $\Delta\beta$ is small. In this case

$$\int_{\beta_0}^{\beta_1} d\beta \hat{C}(\beta)(\beta - \beta_0) \approx \hat{C}(\beta_0) \int_{\beta_0}^{\beta_1} (\beta - \beta_0) = \frac{1}{2}\hat{C}(\beta_0)\Delta\beta^2$$

and

$$\int_{\beta_2}^{\beta_1} d\beta \hat{C}(\beta)(\beta - \beta_2) \approx \hat{C}(\beta_2) \int_{\beta_0}^{\beta_1} (\beta - \beta_2) = \frac{1}{2}\hat{C}(\beta_0)\Delta\beta^2$$

We obtain the simpler expression

$$\mathcal{F}(\beta_0, \beta_1) = \hat{C}(\beta_0)\Delta\beta^2.$$

Thus the condition for errors to be small is

$$\hat{C}(\beta_0)\Delta\beta^2 \ll 1 \qquad |\Delta\beta| \ll \frac{1}{\sqrt{\hat{C}(\beta_0)}},$$

which is the one that we have obtained before, with the more qualitative argument.

It is important to stress that the formula we have obtained has mostly a pure theoretical interest, as it applies asymptotically, when the number of iterations n is so large that $\sigma^2_{\rm est}$ is small. In practical applications, one should use a more robust method, like the jackknife method. Moreover, the jackknife method also allows one to take into account some of the bias, which may be relevant here, as it is also proportional to $\exp \mathcal{F}(\beta_1, \beta_0)$.

The calculation of the error on free energy differences is completely analogous. The computation requires the estimation of $-\ln\langle e^{-\Delta\beta H}\rangle_0$. The corresponding error σ is (we use the error propagation formula, assuming data to be independent)

$$n\sigma^2 = \frac{\langle e^{-2\Delta\beta H}\rangle_0 - \langle e^{-\Delta\beta H}\rangle_0^2}{\langle e^{-\Delta\beta H}\rangle_0^2} = \frac{\langle e^{-2\Delta\beta H}\rangle_0}{\langle e^{-\Delta\beta H}\rangle_0^2} - 1 = e^{\mathcal{F}(\beta_0,\beta_1)} - 1,$$

where n is the number of independent measurements. If data are correlated we only need to introduce the appropriate autocorrelation time. For this quantity it is also easy to compute the bias assuming data to be independent. Prove that

$$\text{bias} \sim \frac{1}{n}(e^{\mathcal{F}(\beta_0,\beta_1)} - 1)$$