Appendix

A Second order numerical integrator

We wish to evaluate

$$I = \int_a^b f(x)dx \tag{A.1}$$

numerically. In order to do it, we construct a numerical integrator up to second order. Let us consider a lattice of N points separated by a length Δx, with the condition $f(x_1) = f(a)$, $f(x_N) = f(b)$. For the interior points of the lattice, we can express the second derivative as

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}. \tag{A.2}$$

where we denote $f_i \equiv f(x_i)$. If N is an odd number, then (A.1) can be written, up to second order, by using a Taylor series

$$I = \sum_{i=1}^{\frac{N-1}{2}} \int_{x_{2i}-\Delta x}^{x_{2i}+\Delta x} \left[f_{2i} + f_{2i}'(x - x_{2i}) + f_{2i}'' \frac{(x - x_{2i})^2}{2} \right] dx, \tag{A.3}$$

where we are only integrating on the even sites. Simplifying eq. (A.3) yields

$$I = \sum_{i=1}^{\frac{N-1}{2}} 2\Delta x f_{2i} + \frac{\Delta x^3}{3} f_{2i}''. \tag{A.4}$$

If we substitute eq. (A.2) we obtain an expression that allows us to evaluate eq. (A.1) when N is odd

$$I = \sum_{i=1}^{\frac{N-1}{2}} \frac{\Delta x}{3} \left(f_{2i+1} + 4f_{2i} + f_{2i-1} \right). \tag{A.5}$$

On the other hand, if N is an even number, we can use the following version of eq. (A.5)

$$I = \sum_{i=1}^{\frac{N}{2}-1} \frac{\Delta x}{3} \left(f_{2i+2} + 4f_{2i+1} + f_{2i} \right). \tag{A.6}$$

However, we still need to integrate from the site x_1 to x_2 (see figure 1 for a graphical depiction). In this case, eq. (A.2) is not valid for the derivatives. Thus, we use the following discretization for the derivatives (see e.g. ref. [1])

$$f_1' = \frac{-3f_1 + 4f_2 - f_3}{2\Delta x}, \quad f_1'' = \frac{2f_1 - 5f_2 + 4f_3 - f_4}{\Delta x^2}. \tag{A.7}$$

Then, the contribution of the interval $[x_1, x_1 + \Delta x]$ to the integral is

$$\begin{aligned}\int_{x_1}^{x_1+\Delta x}\left[f_1+f_1'(x-x_1)+f_1''\frac{(x-x_1)^2}{2}\right] &= f_1\Delta x+\frac{f_1'}{2}\Delta x^2+\frac{f_1''}{6}\Delta x^3\\ &= \Delta x\left(\frac{7}{12}f_1+\frac{1}{6}f_2+\frac{5}{12}f_3-\frac{1}{6}f_4\right). \qquad \text{(A.8)}\end{aligned}$$

Therefore, the general result for the second order numerical integral reads

$$I=\begin{cases}\sum_{i=1}^{\frac{N-1}{2}}\frac{\Delta x}{3}\left(f_{2i+1}+4f_{2i}+f_{2i-1}\right) & \text{for odd } N\\ \sum_{i=1}^{\frac{N}{2}-1}\frac{\Delta x}{3}\left(f_{2i+2}+4f_{2i+1}+f_{2i}\right)\Delta x\left(\frac{7}{12}f_1+\frac{1}{6}f_2+\frac{5}{12}f_3-\frac{1}{6}f_4\right) & \text{for even } N.\end{cases} \qquad \text{(A.9)}$$

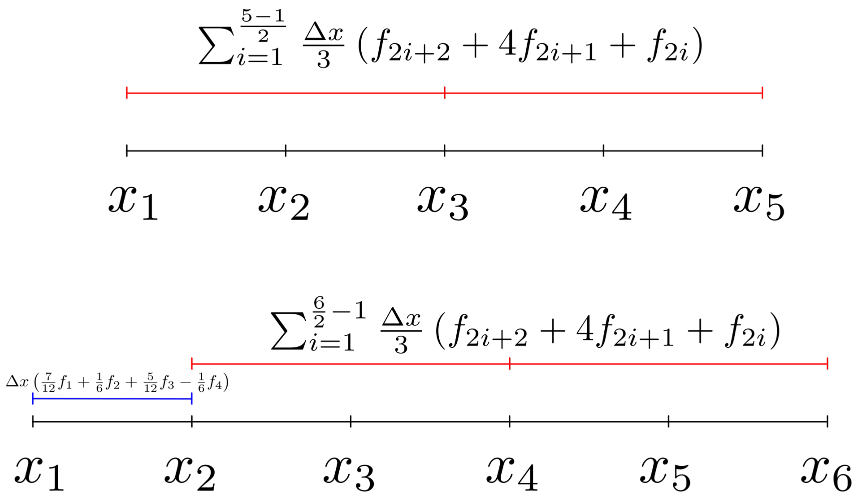

Figure 1: In the upper image we show a lattice with an odd number of points, where we can see that by integrating only in the even sites from $x_{2i} - \Delta x$ to $x_{2i} + \Delta x$, we can compute the numerical integral. In the lower image we show the case of a lattice with even N. There, we can compute the integral from x_2 up to the last site (x_6 in the figure); however, the contribution from x_1 to x_2 would be missing if we only use eq. (A.6). For that reason, one has to use eqs. (A.7) to calculate the contribution from the blue region, which is given by eq. (A.8).

B Jackknife error

The Jackknife error, σ_J, is a special kind of error that allows us to compute the uncertainty of a set of measurements by taking into account possible correlations between them. Let us suppose that we have N measurements of a variable x, we describe σ_J construction as a recipe:

- We calculate the average $\langle x\rangle$ of the N measurements.
- We divide the N measurements in M blocks. M should preferably be a number that satisfies $N/M \in \mathbb{Z}$.
- For each block $m = 1 \dots M$, we consider the set of the N measurements without the block m and calculate its average $\langle x\rangle_m$.
- The Jackknife error is defined as follows

$$\sigma_J=\sqrt{\frac{M-1}{M}\sum_{m=1}^{M}\left(\langle x\rangle_m-\langle x\rangle\right)^2}. \qquad \text{(B.1)}$$

An important remark is that when $M = N$, σ_J coincides with the standard error, since for that case we have

$$\langle x\rangle_m = \frac{1}{N-1}\sum_{m'\neq m}^{N} x_m \Rightarrow \langle x\rangle_m - \langle x\rangle = \frac{1}{N-1}\langle x\rangle - x_m. \tag{B.2}$$

Then

$$\sigma_J = \sqrt{\frac{N-1}{N(N-1)^2}\sum_{m=1}^{N}(x_m - \langle x\rangle)^2} = \sqrt{\frac{1}{N(N-1)}\sum_{m=1}^{N}(x_m - \langle x\rangle)^2}. \tag{B.3}$$

In general, σ_J changes for a different number of blocks M. Due to that, normally one chooses the biggest σ_J for all possible M. Otherwise, the number of blocks has to be specified.

C Autocorrelation time

The autocorrelation time is a quantitative measurement of the correlation between the Monte Carlo configurations. It depends on a specific observable X, the lattice parameters and the algorithm that was used. To define it, we make use of the autocorrelation function

$$C_X(t) = \langle X_i X_{i+t}\rangle - \langle X_i\rangle\langle X_{i+t}\rangle, \tag{C.1}$$

where $t = |i-j|$, $i, j = 1, \ldots N$, with N the number of measurements of X. For large t, the following behavior is known

$$C_X(t) \propto e^{-t/\tau_{\text{exp}}}, \tag{C.2}$$

where we refer to τ_{exp} as the *exponential autocorrelation time.* τ_{exp} can be obtained by measuring $C_X(t)$ for large t and fitting eq. (C.2). A small τ_{exp} means that the configurations are well decorrelated from each other. When that is not the case, it is recommendable to increment the number of sweeps between each configuration that is used to take measurements.

There is another autocorrelation time that can be defined, known as the *integrated autocorrelation time*

$$\tau_{\text{int}} = \frac{1}{2} + \sum_{t=1}^{N}\frac{C_X(t)}{C_X(0)}. \tag{C.3}$$

It can be proved that for large N, the statistical error σ_X is related to the variance

$$\text{Var} = \langle X - \langle X\rangle^2\rangle \tag{C.4}$$

by

$$\sigma_X^2 = 2\tau_{\text{int}}\frac{\text{Var}}{N}. \tag{C.5}$$

Thus, τ_{int} provides a way of finding an error that takes into account correlations between measurements. However, one can use the Jackknife error to do that; so instead it is possible to calculate τ_{int} with (C.5) by substituting $\sigma_J = \sigma_X$. One would expect that this result for τ_{int} coincides with eq. (C.3). See refs. [2, 3, 4] for further details.

Bibliography

[1] B. Fornberg. Generation of finite difference formulas on arbitrarily spaced grids. *Math. Comp.*, 51(184):699–699, 1988.

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