

# Appendix

## A Hybrid Monte Carlo algorithm

In Chapter 2 we described how to implement the Metropolis algorithm to update a scalar field configuration  $[\Phi]$  in order to achieve configurations distributed according to  $p \propto \exp(-S[\Phi])$ , where  $S[\Phi]$  is the discretized Euclidean action. To update the configuration from  $[\Phi]$  to  $[\Phi']$  with this algorithm, one performs local updates  $\Phi_x \rightarrow \Phi'_x$  which are accepted based on the change in the action  $\Delta S[\Phi, \Phi'] = S[\Phi'] - S[\Phi]$ . In many situations,  $\Delta S[\Phi, \Phi']$  only depends on the local update  $\Phi_x \rightarrow \Phi'_x$ , making it cheap to compute. Nevertheless, if we consider gauge fields interacting with fermions, the change in the action

$$\Delta S = S[\psi, \bar{\psi}, U] - S[\psi', \bar{\psi}', U'], \quad (\text{A.1})$$

where  $\psi, \bar{\psi}$  are Grassmann fields and where  $U$  denotes the link variables, does not depend only on local changes. In this case, algorithms that perform local updates require more computing time, since one has to consider the complete configuration to calculate  $\Delta S$  so one can change the value in one site. Several algorithms that update entire configurations by computing  $\Delta S$  just one time have been introduced. In particular, we focus on the Hybrid Monte Carlo (HMC) algorithm [1], which introduces auxiliary momenta  $\pi$ , distributed according to  $p[\pi] \propto \exp(-\pi^2/2)$ , conjugated to the link variables  $U$ . By solving the Hamilton equations we can evolve  $(\pi, U)$  to  $(\pi', U')$  along  $N$  steps over a trajectory in the phase space. This is known as molecular dynamics evolution. After the  $N$  steps, one performs a *Langevin step*<sup>1</sup>, that is, the momenta are generated again and the molecular dynamics evolution is repeated. We describe the HMC procedure for a scalar field. The steps are the same for the implementation in QED; however, it involves a more subtle treatment of the fermion fields and the link variables, which is reviewed in refs. [3–5].

Let us suppose a scalar field configuration  $[\Phi]$  with Euclidean action  $S[\Phi]$ . By introducing the conjugate momenta

$$\pi_x = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}_x}, \quad (\text{A.2})$$

the Hamiltonian is given by

$$H[\Phi, \pi] = \frac{1}{2}\pi^2 + S[\Phi], \quad (\text{A.3})$$

where  $\pi^2 = \sum_x \pi_x^2$  and where  $x$  runs over all the lattice sites. The momentum configuration is generated with a Gaussian distribution

$$p[\pi] \propto e^{-\frac{1}{2}\pi^2} \quad (\text{A.4})$$

and  $[\Phi]$  with a cold or hot start. From eq. (2.42), we know that expectation value of an

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<sup>1</sup>This comes from another algorithm, known as Langevin algorithm (see for instance ref. [2]). Mixing this step with molecular dynamics is the reason of the “hybrid” name.

observable  $A$  is given by

$$\langle A \rangle = \frac{\int \mathcal{D}[\Phi] e^{-S[\Phi]} A[\Phi]}{\int \mathcal{D}[\Phi] e^{-S[\Phi]}}, \quad \mathcal{D}[\Phi] = \prod_x \Phi_x. \quad (\text{A.5})$$

We can insert the momentum to this expression without modifying its final outcome

$$\langle A \rangle = \frac{\int \mathcal{D}[\Phi] \mathcal{D}[\pi] e^{-\frac{1}{2}\pi^2} e^{-S[\Phi]} A[\Phi]}{\int \mathcal{D}[\Phi] \mathcal{D}[\pi] e^{-\frac{1}{2}\pi^2} e^{-S[\Phi]}}, \quad \mathcal{D}[\pi] = \prod_x \pi_x. \quad (\text{A.6})$$

Now, we evolve  $\Phi_x$  and  $\pi_x$  along a trajectory, parametrized by  $\tau$ , with the Hamilton equations

$$\frac{d\Phi_x}{d\tau} = \frac{\partial H}{\partial \pi_x} = \pi_x, \quad \frac{d\pi_x}{d\tau} = -\frac{\partial H}{\partial \Phi_x} = -\frac{\partial S}{\partial \Phi_x}. \quad (\text{A.7})$$

After  $N\Delta\tau$  steps, the system arrives to a new configuration  $(\pi', \phi')$ . As we mentioned in Chapter 2, the detailed balance condition

$$\frac{W([\Phi] \rightarrow [\Phi'])}{W([\Phi'] \rightarrow [\Phi])} = \frac{p[\Phi']}{p[\Phi]} = \frac{e^{-S[\Phi']}}{e^{-S[\Phi]}}, \quad p[\Phi] \propto e^{-S[\Phi]} \quad (\text{A.8})$$

has to be fulfilled. We will show that the condition is satisfied when the transitions are reversible, *i.e.* if we can go from  $(\pi, \Phi)$  to  $(\pi', \Phi')$  with the same probability as from  $(-\pi', \Phi')$  to  $(-\pi, \Phi)$ , and when the measure does not change  $\mathcal{D}[\Phi]\mathcal{D}[\pi] = \mathcal{D}[\Phi']\mathcal{D}[\pi']$ . Since eqs. (A.7) are deterministic, there is a transformation rule

$$f(\pi, \Phi) = (\pi', \Phi') \quad (\text{A.9})$$

that maps  $(\pi, \Phi) \rightarrow (\pi', \Phi')$  and reversibility means that

$$f(\pi, \Phi) = (\pi', \Phi') \Leftrightarrow f(-\pi', \phi') = (-\pi, \phi). \quad (\text{A.10})$$

Both conditions can be achieved numerically by solving eqs. (A.7) with the so-called *leapfrog integrator*, which we describe below.

The Hamiltonian is a constant of motion and the configurations are constrained to  $H = H[\Phi, \pi]$ ; so, in principle,  $(\pi', \Phi')$  could be used as the new configuration of the Markov chain. However, eqs. (A.7) cannot be solved exactly, thus  $H[\Phi, \pi] \neq H[\Phi', \pi']$ . A way to correct this defect is to apply a Metropolis step, *i.e.* to calculate  $\Delta H = H[\Phi', \pi'] - H[\Phi, \pi]$  and only accept the change  $(\pi, \Phi) \rightarrow (\pi', \Phi')$  when  $\Delta H \leq 0$ , or if  $\Delta H > 0$ , accept it with probability  $\exp(-\Delta H)$ .

The leapfrog integrator updates the values of  $\Phi_x$  and  $\pi_x$  in a trajectory of length  $N\Delta\tau$ ,  $N \in \mathbb{N}$ , by evolving the value of  $\Phi_x$  in  $N$  steps of size  $\Delta\tau$  and evolving  $\pi_x$  in  $N$  steps conformed by two intermediate steps of length  $\Delta\tau/2$

$$\begin{aligned} \Phi_x[(i-1)\Delta\tau] &\longrightarrow \Phi_x(i\Delta\tau), \\ \pi_x[(i-1)\Delta\tau] &\rightarrow \pi_x[(i-\frac{1}{2})\Delta\tau] \rightarrow \pi_x(i\Delta\tau), \quad i = 1, \dots, N. \end{aligned} \quad (\text{A.11})$$

The equations for updating the values are

$$\begin{aligned} \Phi_x(i\Delta\tau) &= \Phi_x[(i-1)\Delta\tau] + \Delta\tau \frac{d\Phi_x}{d\tau} \Big|_{\tau=(i-1/2)\Delta\tau}, \\ \pi_x \left[ \left( i - \frac{1}{2} \right) \Delta\tau \right] &= \pi_x[(i-1)\Delta\tau] + \frac{\Delta\tau}{2} \frac{d\pi_x}{d\tau} \Big|_{\tau=(i-1)\Delta\tau}, \\ \pi_x(i\Delta\tau) &= \pi_x \left[ \left( i - \frac{1}{2} \right) \Delta\tau \right] + \frac{\Delta\tau}{2} \frac{d\pi_x}{d\tau} \Big|_{\tau=i\Delta\tau}. \end{aligned} \quad (\text{A.12})$$

We can substitute the derivatives by using eqs. (A.7) and combine eqs. (A.12) to obtain

$$\begin{aligned}\Phi_x(i\Delta\tau) &= \Phi_x[(i-1)\Delta\tau] + \Delta\tau \pi_x[(i-1)\Delta\tau] - \frac{\Delta\tau^2}{2} \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x[(i-1)\Delta\tau]}, \\ \pi_x(i\Delta\tau) &= \pi_x[(i-1)\Delta\tau] - \frac{\Delta\tau}{2} \left[ \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x(i\Delta\tau)} \right].\end{aligned}\quad (\text{A.13})$$

Let us revise that the Jacobian of the transformation  $(\Phi_x[(i-1)\Delta\tau], \pi_x[(i-1)\Delta\tau]) \rightarrow (\Phi_x(i\Delta\tau), \pi_x(i\Delta\tau))$  is equal to one. A computation of the matrix derivative of eqs. (A.13) yields

$$J = \det \begin{pmatrix} 1 - \frac{\Delta\tau^2}{2} \frac{\partial}{\partial \Phi_x[(i-1)\Delta\tau]} \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x[(i-1)\Delta\tau]} & \Delta\tau \\ -\frac{\Delta\tau}{2} \frac{\partial}{\partial \Phi_x[(i-1)\Delta\tau]} \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x[(i-1)\Delta\tau]} & 1 \end{pmatrix} = 1. \quad (\text{A.14})$$

Thus, the measure does not change in any integration step  $i-1 \rightarrow i$ . Since the Jacobian of the transformation from  $\tau = 0$  to  $\tau = N\Delta\tau$  is the multiplication of all the Jacobians of eqs. (A.13) for  $i = 1, \dots, N$ , we conclude that the measure does not change after  $N$  steps, *i.e.*  $\mathcal{D}[\Phi]\mathcal{D}[\pi] = \mathcal{D}[\Phi']\mathcal{D}[\pi']$ .

On the other hand, to show the reversibility we identify eqs. (A.13) as the transformation rule  $f$  that we mentioned in eq. (A.9). To check eq. (A.10) we interchange

$$\Phi_x[(i-1)\Delta\tau] \leftrightarrow \Phi_x(i\Delta\tau), \quad \pi_x[(i-1)\Delta\tau] \leftrightarrow -\pi_x(i\Delta\tau) \quad (\text{A.15})$$

on the right-hand side of eqs. (A.13)

$$\begin{aligned}\Phi_x(i\Delta\tau) - \Delta\tau \pi_x(i\Delta\tau) - \frac{\Delta\tau^2}{2} \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x(i\Delta\tau)} &= \Phi_x(i\Delta\tau) - \Delta\tau \pi_x[(i-1)\Delta\tau] \\ &\quad + \frac{\Delta\tau^2}{2} \left[ \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x(i\Delta\tau)} \right] - \frac{\Delta\tau^2}{2} \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x(i\Delta\tau)} \\ &= \Phi_x(i\Delta\tau) - \Delta\tau \pi_x[(i-1)\Delta\tau] \\ &\quad + \frac{\Delta\tau^2}{2} \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x[(i-1)\Delta\tau]} \\ &= \Phi_x[(i-1)\Delta\tau] \\ -\pi_x(i\Delta\tau) - \frac{\Delta\tau}{2} \left[ \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x[(i-1)\Delta\tau]} + \frac{\partial S}{\partial \Phi_x} \Big|_{\Phi_x(i\Delta\tau)} \right] &= -\pi_x[(i-1)\Delta\tau].\end{aligned}\quad (\text{A.16})$$

Therefore eq. (A.10) is established.

Now, we still have to show that the HMC algorithm obeys detailed balance. But first, let us summarize the algorithm steps as a recipe

1. We generate an auxiliary momentum configuration  $[\pi]$  distributed according to  $p[\pi] \propto \exp(-\sum_x \pi_x^2/2)$ .
2. Then, we solve the Hamilton equations (A.7) by using the leapfrog integrator in order to evolve the system from  $(\pi, \phi) \rightarrow (\pi', \phi')$ .
3. If  $\Delta H = H[\pi', \phi'] - H[\pi, \phi] \leq 0$  the configuration is updated, otherwise the update  $(\pi, \phi) \rightarrow (\pi', \phi')$  is accepted only with probability  $\exp(-\Delta H)$ . This is equivalent to accepting the change with probability  $W_M = \min(1, \exp(-\Delta H))$ .

These three steps are repeated the required number of times and together they conform a sweep. It is important to mention that for each new sweep, the momentum configuration has to be generated again.

To demonstrate detailed balance, we begin with the transition probability to move from  $[\Phi]$  to  $[\Phi']$

$$W(\Phi'|\Phi) = \int \mathcal{D}[\pi]\mathcal{D}[\pi'] W_M(\pi', \Phi'|\pi, \Phi)W_R(\pi', \Phi'|\pi, \Phi)e^{-\pi^2/2}, \quad (\text{A.17})$$

where we introduced the simplified notation  $W(A|B)$ , which means “the probability to move from  $B$  to  $A$ ” (compare for instance with the notation in eq. (A.8)); where  $W_R$  stands for the probability to evolve the system from  $(\pi', \Phi')$  to  $(\pi, \Phi)$ , which satisfy reversibility  $W_R(\pi', \Phi'|\pi, \Phi) = W_R(-\pi, \Phi|-\pi', \Phi')$ , and where  $W_M$  is the probability to accept the update (step 3 of the recipe). We can rewrite  $W_M(\pi', \Phi'|\pi, \Phi)$  as follows

$$\begin{aligned} W_M(\pi', \Phi'|\pi, \Phi) &= \min(1, \exp(-\Delta H)) = \exp(-\Delta H) \min(\exp(\Delta H), 1) \\ &= \exp(-\Delta H)W_M(\pi, \Phi|\pi', \Phi'). \end{aligned} \quad (\text{A.18})$$

Since  $H$  does not depend on the sign of  $\pi$ , we have the relation

$$W_M(\pi', \Phi'|\pi, \Phi) = \exp(-\Delta H)W_M(-\pi, \Phi|-\pi', \Phi'). \quad (\text{A.19})$$

Then

$$\begin{aligned} W(\Phi'|\Phi) &= \int \mathcal{D}[\pi]\mathcal{D}[\pi'] W_M(\pi', \Phi'|\pi, \Phi)W_R(\pi', \Phi'|\pi, \Phi)e^{-\pi^2/2} \\ &= \int \mathcal{D}[\pi]\mathcal{D}[\pi'] e^{-\Delta H}W_M(-\pi, \Phi|-\pi', \Phi')W_R(-\pi, \Phi|-\pi', \Phi')e^{-\pi^2/2} \\ &= \int \mathcal{D}[\pi]\mathcal{D}[\pi'] W_M(-\pi, \Phi|-\pi', \Phi')W_R(-\pi, \Phi|-\pi', \Phi')e^{-S[\Phi'] + S[\Phi] - \pi'^2/2}. \end{aligned} \quad (\text{A.20})$$

Under sign flip  $\pi \rightarrow -\pi$ ,  $\pi' \rightarrow -\pi'$  the measure does not change, therefore

$$\begin{aligned} W(\Phi'|\Phi) &= \int \mathcal{D}[\pi]\mathcal{D}[\pi'] W_M(\pi, \Phi|\pi', \Phi')W_R(\pi, \Phi|\pi', \Phi')e^{-S[\Phi'] + S[\Phi] - \pi'^2/2} \\ &= W(\Phi|\Phi')e^{-S[\Phi'] + S[\Phi]}. \end{aligned}$$

Hence

$$\frac{W(\Phi'|\Phi)}{W(\Phi|\Phi')} = \frac{e^{-S[\Phi']}}{e^{-S[\Phi]}} = \frac{p[\Phi']}{p[\Phi]}, \quad (\text{A.21})$$

*i.e.* detailed balance is satisfied.

## B Second order numerical integral

In Chapter 3 we have to evaluate several integrals of the form

$$I = \int_a^b f(x) dx \quad (\text{B.1})$$

to solve the equations obtained by Hosotani. In order to do so, we construct a numerical integral up to second order. Let us consider a lattice of  $N$  points separated by a length  $\Delta x$ , with the condition  $f(x_1) = f(a)$ ,  $f(x_N) = f(b)$ . For the interior points of the lattice, we can approximate the second derivative as

$$f''_i \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}. \quad (\text{B.2})$$

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

$$I \approx \sum_{i=1}^{\frac{N-1}{2}} \int_{x_{2i}-\Delta x}^{x_{2i}+\Delta x} \left[ f_{2i} + f'_{2i}(x - x_{2i}) + f''_{2i} \frac{(x - x_{2i})^2}{2} \right] dx, \quad (\text{B.3})$$

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

$$I \approx \sum_{i=1}^{\frac{N-1}{2}} 2\Delta x f_{2i} + \frac{\Delta x^3}{3} f''_{2i}. \quad (\text{B.4})$$

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

$$I \approx \sum_{i=1}^{\frac{N-1}{2}} \frac{\Delta x}{3} (f_{2i+1} + 4f_{2i} + f_{2i-1}). \quad (\text{B.5})$$

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

$$I \approx \sum_{i=1}^{\frac{N}{2}-1} \frac{\Delta x}{3} (f_{2i+2} + 4f_{2i+1} + f_{2i}). \quad (\text{B.6})$$

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. (B.2) is not valid for the derivatives, because we do not have any more points to the left of the grid. Thus, we use the following discretization for the derivatives (see e.g. ref. [6]), which only relies on forward steps

$$f'_1 \approx \frac{-3f_1 + 4f_2 - f_3}{2\Delta x}, \quad f''_1 \approx \frac{2f_1 - 5f_2 + 4f_3 - f_4}{\Delta x^2}. \quad (\text{B.7})$$

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

$$\begin{aligned} \int_{x_1}^{x_1+\Delta x} \left[ f_1 + f'_1(x - x_1) + f''_1 \frac{(x - x_1)^2}{2} \right] dx &= f_1 \Delta x + \frac{f'_1}{2} \Delta x^2 + \frac{f''_1}{6} \Delta x^3 \\ &= \Delta x \left( \frac{7}{12} f_1 + \frac{1}{6} f_2 + \frac{5}{12} f_3 - \frac{1}{6} f_4 \right). \end{aligned} \quad (\text{B.8})$$

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

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

We can test the result with the following definite integrals

$$\int_0^\infty e^{-x^2} dx = \frac{\sqrt{\pi}}{2}, \quad \int_0^\pi e^x \cos(x) dx = -\frac{1}{2}(1 + e^\pi). \quad (\text{B.10})$$

In figure 2 we show the numerical value of these integrals as a function of the number of points,  $N$ , on the lattice. We see that the result converges to the right value.

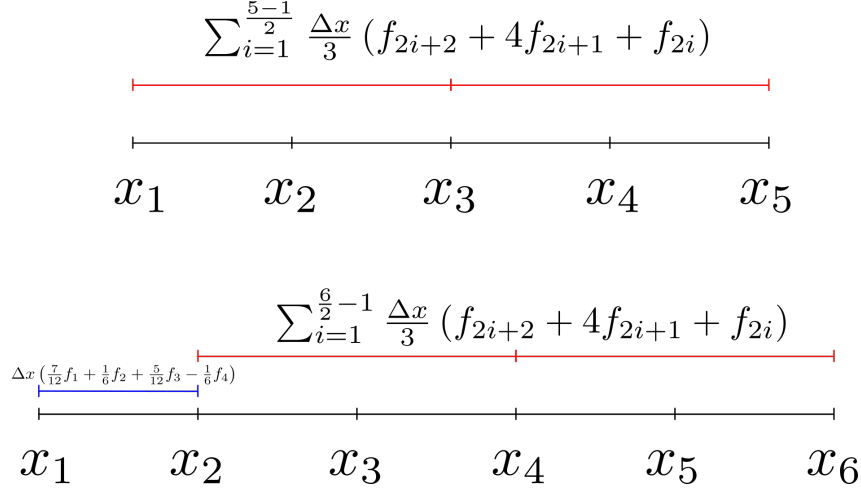
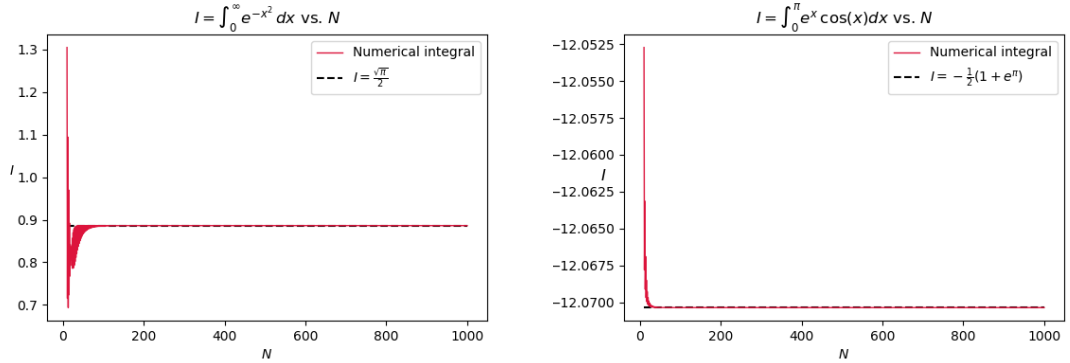


Figure 1: In the upper image we show a lattice with an odd number of points, where we can see that by integrating only in the even sites from  $x_{2i} - \Delta x$  to  $x_{2i} + \Delta x$ , we can compute the numerical integral. In the lower image we show the case of a lattice with even  $N$ . There, 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. (B.6). For that reason, we have to use eqs. (B.7) to calculate the contribution from the blue region, which is given by eq. (B.8).



(a)  $\int_0^\infty e^{-x^2} dx$  as a function of the number of points used to evaluate the integral. (b)  $\int_0^\pi e^x \cos(x) dx$  as a function of the number of points used to evaluate the integral.

Figure 2: Test of the convergence of the numerical integral with the examples of eq. (B.10).

## C Jackknife error

The jackknife error  $\sigma_J$ , is a special kind of error that allows us to compute the uncertainty of a set of measurements by taking into account possible autocorrelations between them. It is also useful to determine the error of a fit parameter. For instance, an error to the energy gap given by the correlation function (eq. (2.44)) can be obtained by fitting a cosh function to several data subsets and by estimating  $\sigma_J$ , using the resultant parameter of each fit as a measurement.

Let us suppose that we have  $N$  measurements of a variable  $x$ . We describe the calculation of  $\sigma_J$  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  $N/M \in \mathbb{N}$ .

- 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

$$\sigma_J = \sqrt{\frac{M-1}{M} \sum_{m=1}^M (\langle x \rangle_m - \langle x \rangle)^2}. \quad (\text{C.1})$$

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

$$\langle x \rangle_m = \frac{1}{N-1} \sum_{m' \neq m}^N x_{m'} \implies \langle x \rangle_m - \langle x \rangle = \frac{1}{N-1} (\langle x \rangle - x_m). \quad (\text{C.2})$$

Then

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

In general,  $\sigma_J$  changes for a different number of blocks  $M$  and it tends to be larger than the standard error. Due to that, normally one calculates the right-hand side of eq. (C.1) for several  $M$  and chooses the error as the largest value of the  $\sigma_J$  that were computed.

## D Autocorrelation time

The autocorrelation time is a quantitative measure of the autocorrelation between the Markov chain configurations. It depends on a specific observable  $X$ . To define it, we make use of the correlation function

$$C_X(t) = \langle X_i X_{i+t} \rangle - \langle X_i \rangle \langle X_{i+t} \rangle, \quad (\text{D.1})$$

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

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

where we refer to  $\tau_{\text{exp}}$  as the *exponential autocorrelation time*.  $\tau_{\text{exp}}$  can be obtained by measuring  $C_X(t)$  for large  $t$  and fitting eq. (D.2). A small  $\tau_{\text{exp}}$  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*

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

It can be proved that for large  $N$  (see e.g. ref. [7]), the statistical error  $\sigma_X$  is related to the decorrelated variance

$$\text{Var} = \langle X - \langle X \rangle^2 \rangle \quad (\text{D.4})$$

by

$$\sigma_X^2 = 2\tau_{\text{int}} \frac{\text{Var}}{N}. \quad (\text{D.5})$$

Thus,  $\tau_{\text{int}}$  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  $\tau_{\text{int}}$  with eq. (D.5) by substituting  $\sigma_J = \sigma_X$ . Another application of eq. (D.5) is that it tells us that we are using an effective sample of  $N/(2\tau_{\text{int}})$  measurements. If  $\tau_{\text{int}} = 1/2$ , the effective sample is  $N$ , which indicates a perfect decorrelation. This is motivated by the fact that with decorrelated data the uncertainty is simply the standard error  $\sqrt{\text{Var}/N}$ . A deeper discussion about the autocorrelation time can be found in refs. [8, 9].



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