The Les Houches Recitations: Day 4
Stefan Schaefer, Humboldt Universität zu Berlin

1 Error Analysis

Most Monte Carlo algorithms produce a series of field configurations which are correlated among each other. These correlations die out with increasing Monte Carlo time separation, however, it still poses a problem to the estimation of the statistical errors of measured observables. To be specific, our algorithm produces configurations $\phi^1 \to \phi^2 \to \cdots \to \phi^N$ on which observable A^α are measured. So we get a set of measurements $\{A_i^\alpha : i = 1, \ldots, N\}$. Let us assume that the thermalization process is already completed and the ϕ^i are in equilibrium. To quantify the correlations between the successive configurations one looks at the *auto-correlation function* $\Gamma_{\alpha\beta}$

$$\Gamma_{\alpha\beta}(t) = \langle (A_i^\alpha - \langle A^\alpha \rangle)(A_{i+t}^\beta - \langle A^\beta \rangle) \rangle \ .$$

Auto-correlations let this to be non-zero for $t > 0$. The brackets $\langle \cdots \rangle$ mean an average over repeated 'experiments', i.e. independent sets of N configurations. Of course, we almost never do this in real life, but use an estimator from one Markov chain

$$\bar{\Gamma}_{\alpha\beta}(t) \ = \ \frac{1}{N-t} \sum_{i=1}^{N-t} (A_i^\alpha - \bar{A}^\alpha)(A_{i+t}^\beta - \bar{A}^\beta) + \mathcal{O}(1/N) \tag{1}$$

with $\bar{A}^\alpha = \frac{1}{N} \sum_i A_i^\alpha$.
In most lattice simulations we compute observables, which are functions of such averages of primary observables.

$$F = F(A^1, \ldots, A^n)$$

from which we also need the derivatives $f_\alpha = \partial F / \partial A_\alpha$. Then the obvious estimator is $\bar{F} = F(\bar{A}^1, \ldots, \bar{A}^n)$ and its error σ_F is given by[2]

$$\sigma_F^2 = \frac{2\tau_{\text{int}}}{N} v_F$$

with the variance corresponding to F given by

$$v_F = \sum_{\alpha\beta} f_\alpha f_\beta \Gamma_{\alpha\beta}(0)$$

and the integrated auto-correlation time for F

$$\tau_{\text{int},F} = \frac{1}{2} + \frac{1}{v_F} \sum_{t=1}^{\infty} \sum_{\alpha\beta} f_\alpha f_\beta \Gamma_{\alpha\beta}(t)$$
$$\equiv \frac{1}{2} + \sum_{t=1}^{\infty} \rho_F(t)$$

The error of the normalized auto-correlation function ρ can also be given

$$[\delta\rho_F(t)]^2 = \frac{1}{N} \sum_{k=1}^{\infty} (\rho_F(k+t) + \rho_F(k-t) - 2\rho_F(t)\rho_F(k))^2$$

Note that $\rho_F(t) = \rho_F(-t)$.

Because $\Gamma_{\alpha\beta}(t)$ is only poorly determined for large t, the sum for τ_{int} has to be truncated at some finite "window" W. Otherwise one would essentially sum up noise and increase the error of the computed $\tau_{\text{int},F}$.

$$\bar{\tau}_{\text{int},F} = \frac{1}{2} + \sum_{k=1}^{W} \rho_F(t) \ . \tag{2}$$

By neglecting the contribution from $k > W$ one introduces a bias in the estimator. According to Madras and Sokal[1], the variance of this estimator, however, of τ_{int} is given by

$$(\delta\tau_{\text{int},F})^2 \approx \frac{4W+2}{N}\tau^2_{\text{int},F} \ ,$$

which shows that without a finite W the variance would be infinite. The right choice of W amounts to a balance between bias and variance of the estimator of τ_{int}[3]. Lüscher in Ref. [4] suggests to sum up to the smallest W such that $\sqrt{\langle\delta\rho(W)^2\rangle} \geq \rho(W)$.

1.1 Tasks

1. If you want, write a program which reads in the MC time history of the observables A^i and computes the expectation value of a derived quantity $\bar{F}$ and its error. Alternatively, get a *simple* implementation at
`http://www-com.physik.hu-berlin.de/~sschaef/LH/gamma.c` .
So far, the function $F(x) = x$ and its derivative are implemented.

2. Take a sample equilibrium history of m and m^2 and compute the normalized auto-correlation functions ρ. Plot them and look at the exponential fall-off. Then compute $\tau_{\text{int}}(W)$ and do some experiments regarding the summation window W. Suggestion: Use $L/a = 6$, $\lambda = 1.145$ and $\kappa = 0.18$ with 10^6 measurements.

3. Study the dependence of the auto-correlation time of m^2 on the trajectory length and the step size. What are issues in choosing it for production running?

4. Now extend the program to analyze the Binder cumulant. Compute the necessary derivatives analytically and modify the `observable()` and `derivative()` routines.

5. In the vicinity of phase transitions auto-correlation times tend to increase for most algorithms. This is called critical slowing down. Study τ_{int} of m and the Binder cumulant as κ crosses the critical point of $\kappa_c = 0.1864463(4)$ at $L/a = 6$, $\lambda = 1.145$.

6. Try to get the exponential auto-correlation time τ_{exp}, for which should hold $\rho(t) = C\exp(-t/\tau_{\text{exp}})$ for $t \to \infty$. (To be more precise, it is the supremum over all possible observables.)

2 Critical exponents

For this section, time is too short, but I left it in for the last step to get "real" numbers.
The theory of critical phenomena tells us, that in the vicinity of criticality, U in the ϕ^4 model shows the following universal behavior

$$U = U^* + c(\lambda)(\kappa - \kappa_{\text{cr}})L^{1/\nu} + d(\lambda)L^{-\omega} + \ldots$$

where we dropped terms which are even stronger suppressed in L. So we can get the critical exponent ν by considering the derivative of U with respect to κ at fixed λ. Dropping the higher terms yields

$$\frac{\partial}{\partial\kappa}U \approx cL^{1/\nu}$$

and we can get ν from the dependence of this quantity on L at fixed λ. This is the more traditional approach to the problem. More modern would be to hold some other observable fixed and thereby eliminate also the non-leading corrections. In the following, we will use $\lambda = 1.145$, $\kappa = 0.1864463$ and perform runs on $L = 4, \ldots, 9$. This value of κ is the estimate of the critical value taken from Ref. [6] which along with Ref. [5] is a good reference for how to do such computations professionally.

2.1 Task

1. Measure the derivative of the Binder cumulant as a function of L and determine ν. To get the derivative, use the method sketched on the first problem sheet.

References

[1] N. Madras and A. D. Sokal, J. Statist. Phys. **50** (1988) 109.

[2] U. Wolff [ALPHA collaboration], Comput. Phys. Commun. **156** (2004) 143 [Erratum-ibid. **176** (2007) 383] [arXiv:hep-lat/0306017].

[3] A. D. Sokal, Monte Carlo Methods in Statistical Mechanics: Foundations and New Algorithms, Lectures ath the Cargeèse Summer School, 1996

[4] M. Lüscher, Comput. Phys. Commun. **165** (2005) 199 [arXiv:hep-lat/0409106].

[5] M. Hasenbusch, K. Pinn and S. Vinti, Phys. Rev. B **59** (1999) 11471.

[6] M. Hasenbusch, J. Phys. A **32** (1999) 4851 [arXiv:hep-lat/9902026].