Efficient Monte Carlo Calculation of the Free Energy in Low Dimensions

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Abstract

A novel approximation technique – the improved Gaussian approximation – developed in the previous publication [1] is used to improve the efficiency of the Monte Carlo calculation of the free energy in low dimensions. As an example, we consider the generic non-linear $q^3 + q^4$ model in $d = 0$ dimensions and obtain a sizeable speed-up over the standard algorithm. The implications for the $d = 1$ case, when the speed-up should be exponential in the number of time slices, are discussed.

In a recent paper [1] we have studied a generic non-linear oscillator model with cubic and quartic couplings:

$$\mathcal{H}(q) = \frac{1}{2}\, q^2 + \frac{1}{3!}\, g_3\, q^3 + \frac{1}{4!}\, g_4\, q^4 \tag{1}$$

in $d = 0$. We have introduced a Gaussian approximation for the partition function

$$Z(B) \equiv e^{-\beta F(B)} = \int dq\, e^{-\beta(\mathcal{H}(q) - B\, q)}\ , \tag{2}$$

and showed that it can be used to generate a sequence of approximations of increasing quality for the free energy $F(B)$ and the magnetization $M = \langle q \rangle = -\frac{\partial}{\partial B} F(B)$. The zero and first order approximations in this scheme correspond to the familiar mean field and semi-classical approximations [2]. The second order approximation, called the improved Gaussian approximation (IGA), was studied in detail, and shown to be superior to the first two.

The aim of our investigations in [1] has been to develop a better analytic approximation scheme that can be applied to general models in statistical mechanics. We worked in $d = 0$ in order to be able to make a simple comparison with exact (numerical) results. In the present paper we go a step further and study the numerical techniques themselves. The method of choice for calculating path integrals featuring in the definition of the partition function is the Monte Carlo (MC) algorithm [3]. Of course, in $d = 0$ MC is not the most efficient method to do the calculation since its advantages become apparent as the number of required integrations grows. We use MC in order to investigate the algorithm

itself in light of what we have learned in [1, 4, 5], and as a stepping stone to a future MC calculation in $d = 1$ and higher.

To clarify the subsequent discussion we start with a brief description of the MC method. In order to calculate the definite integral $\int dq\, f(q)$ we choose a probability distribution $p(q)$, and rewrite the integral as

$$\int dq\, f(q) = \int dq\, \frac{f(q)}{p(q)}\, p(q) \equiv \left\langle \frac{f}{p} \right\rangle_p , \tag{3}$$

where $\langle F \rangle_p$ denotes the mean value of F with respect to the probability distribution p. Therefore, the integral of f is given as the mean value of f/p on a sample of random numbers whose probability distribution is given by p. In practice, this mean value is estimated using a finite number $N_{\rm mc}$ of MC samples, and the error of such an estimate is itself estimated to be $\sigma_{f/p} = \sqrt{\sigma^2_{f/p}}$, where the variance equals

$$\sigma^2_{f/p} = \frac{1}{N_{\rm mc} - 1} \left[\left\langle \left(\frac{f}{p} \right)^2 \right\rangle_p - \left\langle \frac{f}{p} \right\rangle_p^2 \right] . \tag{4}$$

It can be shown that as $N_{\rm mc} \to \infty$, the MC algorithm converges to $\int dq\, f$ for an arbitrary choice of distribution p. The only condition that must be met is $\sigma^2_{f/p} < \infty$ [3]. This freedom of choice can be used to speed-up the convergence of the algorithm. The speed of convergence is measured by the efficiency $\mathcal{E}$, given by

$$\mathcal{E} = \frac{1}{T\, \sigma^2_{f/p}} , \tag{5}$$

where T denotes the total computation time. Note that a hundred fold increase of efficiency corresponds to one extra significant figure in the final result for a fixed amount of computer effort.

In our calculation we chose $p(q)$ to be the Gaussian normal distribution

$$p(q) = \frac{1}{\sqrt{2\pi\sigma^2}}\, \exp\left(- \frac{(q-a)^2}{2\sigma^2} \right) . \tag{6}$$

There are three reasons for this choice. First, the function we are integrating can be approximated by a Gaussian over a wide range of B, g_3, and g_4. A good choice of parameters a and σ makes f/p almost constant over the range of integration, thus making the variance small. Second, there exists a specific algorithm for generating random numbers conforming to a Gaussian distribution. The Box-Muller algorithm [6] is more efficient than the standard Metropolis algorithm [7] since it doesn't give rise to autocorrelations of generated numbers whose presence can substantially slow down the simulation. Last, the use of the Gaussian distribution enables us to apply the insights gained in studies of IGA [1, 4, 5].

The choice of probability distribution has a great effect on the efficiency. For example, the efficiency corresponding to the uniform distribution on the interval $q \in [-100, 100]$ is $3.5\ 10^{10}$ times smaller than the efficiency achieved by the Gaussian distribution centered at the mean field $a = q_{\rm mf}$ with optimal choice of width σ. Let us recall that the mean field $q_{\rm mf}$ is defined by $\mathcal{H}' = B$, i.e. it corresponds to the maximum of the integrand. Having chosen p to be a Gaussian, the computation time T depends only on the number of MC samples $N_{\rm mc}$. Therefore, the maximization of efficiency is, in our case, equivalent to the minimization of the variance $\sigma^2_{f/p}$.

It is apparent that the MC parameter a plays a role analogous to that of q_{ref} in [1] (see equation (3) therein). Therefore, on the basis of the main insight of that work that the Gaussian expansion of the integrand should be done around the magnetization rather than around the mean field solution, we expect that a further gain in efficiency of the MC algorithm can be achieved when p is centered at $M(B)$ rather than at $q_{\rm mf}$. This is *precisely* what we find. By varying the center of the Gaussian a (always using optimal width σ for that given a), we find that the maximum efficiency is reached at $a = M(B)$. Figure 1 illustrates this point for a typical choice of parameters.

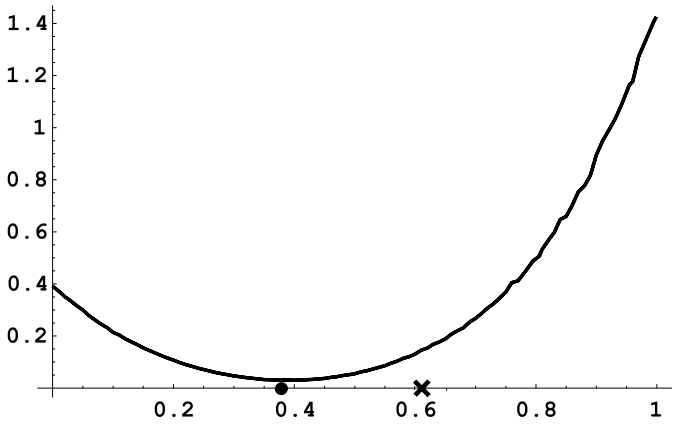

Figure 1: The variance as a function of the parameter a. The plot is for $g_3 = 0$, $g_4 = 10$, $B = 1$, and $\beta = 1$. The variance is minimal for $M(1) = 0.377$ (dot). The mean field solution is $q_{\rm mf}(1) = 0.614$ (cross).

Figure 2 compares the efficiencies $\mathcal{E}_{\rm mf}$ of simulations done using the distribution centered at $q_{\rm mf}$, and $\mathcal{E}_Q$ for those centered at $M(B)$ for various values of B. It is seen that we get a two fold improvement in efficiency. This may not seem spectacular, and in $d = 0$ it really is not. However, once we consider theories in $d > 0$ and deal with true path integrals, this conclusion changes considerably. If the path integral is approximated with N integrals then the expansion around M increases the efficiency $(\mathcal{E}_Q/\mathcal{E}_{\rm mf})^N \approx 2^N$ times. Even for a modest simulation with $N = 20$ this corresponds to an increase of six orders of magnitude.

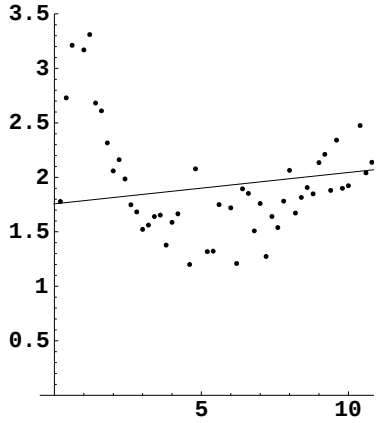

Figure 2: The ratio $\mathcal{E}_Q/\mathcal{E}_{\rm mf}$ as a function of B for $g_3 = 0$, $g_4 = 1$, and $\beta = 1$. The line is a guide for the eye. Similar results are obtained for other values of the couplings g_3 and g_4.

The problem with the above calculation is that we already need to have the exact result for $M(B)$ in order to get the stated increase in speed. The way out is obvious and is reminiscent of the procedure we have adopted in [1]. Thus, we start MC with a Gaussian distribution centered at $q_{\rm mf}$. After a while this gives us an approximation to M, denoted as $M_1^{\rm mc}$. Using this as the center of a new probability distribution we obtain $M_2^{\rm mc}$, etc. Unlike the series of analytical approximations M_0, M_1, $M_2, \ldots$ of the previous paper [1], this one trivially converges to the exact result since its every step does so. The improved MC scheme, however, can be organized in such an adaptive way to yield an efficiency very near to the ideal value $\mathcal{E}_Q$.

In conclusion, we have used the insights gained in previous studies of the improved Gaussian approximation to set up an efficient Monte Carlo procedure for the calculation of the partition function and free energy in $d = 0$. A considerable speed-up, exponential in the number of time slices, is predicted for calculations of path integrals in $d = 1$. A work in that direction is in progress.

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