

Reweighting complex Langevin trajectories

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Although the complex Langevin method can solve the sign problem in simulations of theories with complex actions, the method will yield wrong results if known validity conditions are not satisfied. We present a novel method to compute observables for a target ensemble by reweighting complex trajectories generated with the complex Langevin method for an auxiliary ensemble having itself a complex action. While it is imperative that the validity conditions be satisfied for the auxiliary ensemble, there are no such requirements for the target ensemble. This allows us to enlarge the applicability range of the complex Langevin method. We illustrate this at the hand of a one-dimensional partition function and two-dimensional strong-coupling QCD.

Keywords: Lattice QCD, Quark Chemical Potential, Sign Problem

I. INTRODUCTION

Lattice simulations of quantum chromodynamics (QCD) at nonzero chemical potential are especially challenging as the complex fermion determinant rules out the use of importance sampling methods. Current solutions to circumvent this sign problem have a computational cost which grows exponentially with the volume and are restricted to regions of parameter space which do not encompass the phenomenologically interesting phase transition [1]. An alternative solution method that has attracted a lot of attention recently is the complex Langevin (CL) method [2, 3], which uses stochastic differential equations for complexified degrees of freedom to sample the partition function and compute expectation values. The hope that this method may be used to investigate the QCD phase transition has recently been denied by investigations in heavy-dense [4] and full QCD [1], which seem to indicate that the method has problems in the critical region. This concern has been amplified by recent results in low-dimensional strong-coupling QCD [5] where the method was shown to converge to incorrect result for small masses. It is now understood that the CL method only produces correct results if some definite validity conditions are satisfied, and this is exactly what goes wrong for certain parameter regions of the theories being investigated.

In this paper we introduce the reweighted complex Langevin (RCL) method which combines CL and reweighting to reach regions of parameter space which can otherwise not be reached by the CL method. The principle is simple: we generate a CL trajectory for an auxiliary ensemble with parameter values for which the CL validity conditions are satisfied and then reweight this trajectory of complexified configurations to the target parameter values. One of the upshots of the method is that the validity conditions do not have to be satisfied in the target ensemble.

In contrast to standard reweighting methods, the auxiliary ensemble in this hybrid procedure is taken at parameter values where the action is complex such that it could be closer to the target ensemble, hence making the reweighting more efficient.

The RCL method is generally applicable to theories with complex actions and has now already been tested successfully on a one-dimensional partition function with strong sign problem [6, 7], random matrix models of QCD [8–10] and QCD in 0+1 and 1+1 dimensions [5, 11].

In Section II we give a brief introduction of the complex Langevin method and its validity conditions. In Section III we introduce the reweighted complex Langevin method, which is the main theme of this paper. In Section IV we briefly illustrate the method with results for a one-dimensional partition function and for two-dimensional QCD. Finally we conclude in Section V.

II. COMPLEX LANGEVIN METHOD

Consider a partition function

$$Z = \int dx e^{-S(x)} \quad (1)$$

with multidimensional real degrees of freedom x and a complex action $S(x)$, which leads to the sign problem.

A Langevin equation based on the complex action is driven by a complex force, which naturally takes the real variables into the complex plane. Therefore, we introduce complexified variables $z = x + iy$ satisfying the CL equation

$$\dot{z}(t) = -\frac{\partial S}{\partial z} + \eta(t) \quad (2)$$

with independent multidimensional Gaussian noise η , which is chosen real to get better convergence, satisfying

$$\langle \eta(t) \rangle = 0, \quad \langle \eta(t) \eta(t') \rangle = 2\delta(t - t'). \quad (3)$$

In practice the stochastic differential equations need to be discretized, which in the stochastic Euler scheme

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yields

$$z(t+1) = z(t) + \epsilon K + \sqrt{\epsilon} \eta, \quad (4)$$

with drift term $K = -\partial S/\partial z$ and discretized Langevin step size ϵ .

When applying the complex Langevin method it is essential that the expectation values computed along the complex trajectory agree with the original expectation values in the partition function with complex action, i.e.,

$$\langle \mathcal{O} \rangle \equiv \int dx \rho(x) \mathcal{O}(x) = \int dx dy P(z) \mathcal{O}(z), \quad (5)$$

where $\rho(x) = e^{-S(x)}/Z$ is the complex weight in the original real variables and $P(z)$ is the real probability in the complex variables $z = x + iy$ along the complex Langevin trajectory.

Proving the equivalence (5) has been the object of thorough study in recent years [7, 12], and it is now known to hold if the following validity conditions are satisfied:

- The probability $P(z)$ decays sufficiently rapidly in the imaginary direction of the complexified variables to avoid the *excursion* problem;
- The probability density $P(z)$ is suppressed close to singularities of the drift and of the observable.

Recently it was shown that these conditions can be replaced by the single condition that the probability distribution of the drift term should be suppressed, at least, exponentially at large magnitude [7].

These validity conditions are not always satisfied as was verified for various models and physical systems, in which case the CL method will fail or its expectation values will be incorrect [5–8, 13].

The RCL method proposed below uses reweighting to extend the applicability of the CL method to parameter regions for which the CL validity conditions are not satisfied.

III. REWEIGHTING THE COMPLEX LANGEVIN TRAJECTORIES

The basic principle of the reweighted complex Langevin method (RCL) is to compute observables for a target ensemble by reweighting the complex CL trajectories generated for an auxiliary ensemble. For this, it is imperative that the CL validity conditions are satisfied for the auxiliary ensemble, but it is interesting to note that they may be violated in the target ensemble.

We first introduce the standard reweighting method to compute the expectation value of an observable \mathcal{O} in a target ensemble characterized by the parameters ξ ,

$$\langle \mathcal{O} \rangle_\xi = \frac{\int dx w(x; \xi) \mathcal{O}(x; \xi)}{\int dx w(x; \xi)}, \quad (6)$$

with weights $w(x; \xi) = e^{-S(x; \xi)}$ and action $S(x; \xi)$. To compute this expectation value via reweighting we also consider an auxiliary ensemble with parameter values ξ_0 and rewrite Eq. (6) in a completely equivalent form

$$\langle \mathcal{O} \rangle_\xi = \frac{\int dx w(x; \xi_0) \left[\mathcal{O}(x; \xi) \frac{w(x; \xi)}{w(x; \xi_0)} \right]}{\int dx w(x; \xi_0) \left[\frac{w(x; \xi)}{w(x; \xi_0)} \right]} = \frac{\left\langle \mathcal{O}_\xi \frac{w_\xi}{w_{\xi_0}} \right\rangle_{\xi_0}}{\left\langle \frac{w_\xi}{w_{\xi_0}} \right\rangle_{\xi_0}}. \quad (7)$$

This reweighting equation gives a mathematically exact relation between expectation values in the target ensemble and in an auxiliary ensemble and holds independently of the actions being real or complex.

In standard practice the auxiliary ensemble is chosen with real and positive weights so that it can be sampled with importance sampling Monte Carlo methods and the target observables can be estimated as ratio of sample means according to Eq. (7). The target ensemble can have either a real or complex action. An example of real action reweighting is mass reweighting in QCD. However, the more relevant case here is when the target ensemble has complex weights and can itself not be sampled with importance sampling methods, as is the case in QCD at nonzero chemical potential. Reweighting is then one possible way to circumvent the sign problem.

The peculiarity of the new RCL method is that we drop the requirement for the auxiliary weights to be real and positive and allow these to be complex, i.e., we reweight from one ensemble with complex action to another one with complex action. Although Eq. (7) remains formally correct, this makes a crucial difference from the algorithmic point of view as we can no longer use importance sampling methods to sample relevant configurations in the auxiliary ensemble. Instead we aim to use the CL method to generate an auxiliary trajectory, i.e., a trajectory in the auxiliary ensemble, along which expectation values in that ensemble can be estimated. For these estimates to be correct the auxiliary ensemble has to be chosen such that the CL conditions of Section II are satisfied. If we then consider such an auxiliary CL trajectory, the expectation value of any observable \mathcal{O} in this ensemble can be computed, according to the CL equivalence (5), as

$$\langle \mathcal{O} \rangle_{\xi_0} = \int dx dy P(z; \xi_0) \mathcal{O}(z), \quad (8)$$

where $P(z; \xi_0)$ is the real probability in the complex variable along the auxiliary CL trajectory.

The leap in the RCL method is that we apply the CL formula (8) to both the numerator and denominator of the reweighting equation (7), hereby specifying the observable \mathcal{O} of Eq. (8) to the expressions in square brackets

in Eq. (7). This eventually leads to the RCL equation

$$\langle \mathcal{O} \rangle_\xi = \frac{\int dx dy P(z; \xi_0) \left[\mathcal{O}(z; \xi) \frac{w(z; \xi)}{w(z; \xi_0)} \right]}{\int dx dy P(z; \xi_0) \left[\frac{w(z; \xi)}{w(z; \xi_0)} \right]}. \quad (9)$$

Note that, compared to Eq. (7), the expressions in square brackets are now to be evaluated in the complex variable along the auxiliary CL trajectory. In applying Eq. (8) to the reweighting equation an interesting difference between the RCL method and the standard reweighting procedure arises: in the latter the auxiliary ensemble is sampled according to $w(x; \xi_0)$ and this same factor also occurs in the denominator of the effective observables, whereas in Eq. (9) for RCL the ensemble is sampled according to the real probability $P(z; \xi_0)$ but the effective observables contain the complex weights $w(z; \xi_0)$.

An important observation is that, even if the CL validity conditions are not satisfied for the target ensemble, the RCL equation (9) will still yield the correct result as it only uses expectation values in the auxiliary ensemble where the validity conditions are assumed to be satisfied.

In practice the auxiliary CL trajectory is discretized using Eq. (4), and Eq. (9) is estimated by the ratio of sample means

$$\langle \mathcal{O} \rangle_\xi \approx \frac{\frac{1}{N} \sum_{j=1}^N \mathcal{O}(z_j; \xi) \frac{w(z_j; \xi)}{w(z_j; \xi_0)}}{\frac{1}{N} \sum_{j=1}^N \frac{w(z_j; \xi)}{w(z_j; \xi_0)}}. \quad (10)$$

Although Eq. (7) is mathematically exact, its practical use is subject to caution. When the auxiliary and target ensembles are not close enough the accuracy of the method in numerical simulations is plagued by the overlap and sign problems. The overlap problem already occurs when the weights in both ensembles are positive, while the sign problem occurs additionally when the target weights are complex and large cancellations occur in the integrals.

A possible asset of the RCL procedure is that it may allow us to reweight from an auxiliary ensemble that is *closer* to the target ensemble than in standard reweighting, where the auxiliary ensemble needs to have real and positive weights.

IV. RESULTS

Below we briefly illustrate the RCL method on two examples: a one-dimensional partition function and two-dimensional strong-coupling QCD.

Consider the one-dimensional partition function [6]

$$Z = \int_{-\infty}^{+\infty} dx (x + i\alpha)^4 e^{-x^2/2}, \quad (11)$$

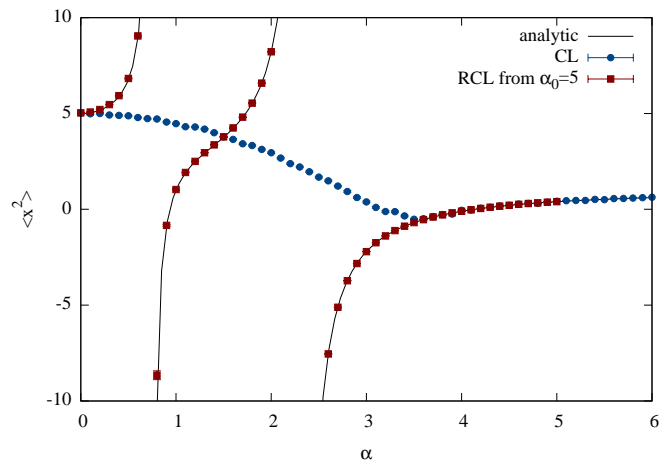


FIG. 1. Results for $\langle x^2 \rangle$ as a function of α for the one-dimensional partition function (11). Comparison of CL (blue), RCL (red) and analytical (solid) results.

for which $\langle x^2 \rangle$ was shown to converge to a wrong solution for a large parameter range using the CL method, as the trajectories cover the singularity of the drift. In Fig. 1 we compare the CL and RCL results for $\langle x^2 \rangle$ with the known analytical results. The CL results are wrong when $\alpha \lesssim 3.4$, however the RCL, using an auxiliary trajectory generated at $\alpha_0 = 5.0$, is able to reproduce the correct results over a very large α -range, even across the discontinuity jumps in the observable.

As second illustration we show results for two-dimensional strong-coupling QCD, for which more details can be found in Ref. [11]. The partition function depends on the chemical potential μ and the quark mass m . The sign problem is triggered by the chemical potential: for zero μ the action is real and there is no sign problem; as μ is increased the action becomes complex and for a certain range of the parameters, especially for small masses, the sign problem can be very strong. Moreover, the sign problem grows exponentially with the lattice volume. Although CL can in principle be used to avoid the sign problem, it was shown in Ref. [5] that for small masses the CL trajectories cover the singularity of the drift such that the CL validity conditions are violated and the CL results are wrong. This can be seen in Fig. 2 where the quark number density is shown as a function of the chemical potential for a small mass, $m = 0.1$, on a 6×6 lattice. In the phase transition region ($\mu \in [0.2, 0.55]$) the CL results clearly disagree with the phase-quenched benchmarks. Reweighting from $\mu_0 = 0.6$ using RCL rectifies this situation and agreement is achieved, within the somewhat larger error bars, over the complete μ -range.

In both examples RCL is able to reproduce the correct results, even when CL fails for the target ensemble. In separate publications we present more detailed RCL results obtained for a random matrix model of QCD [10] and for two-dimensional QCD [11].

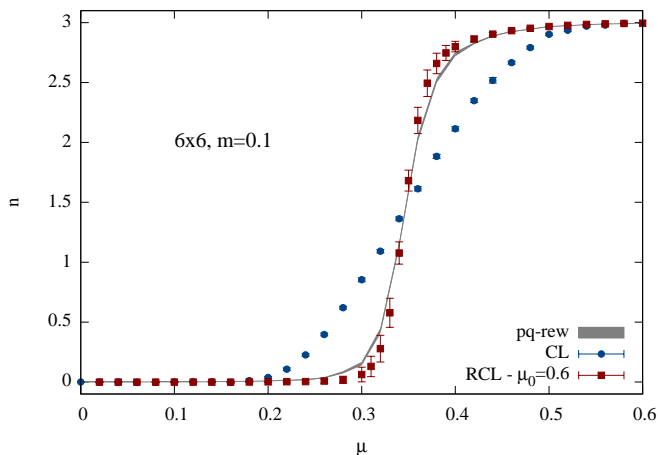


FIG. 2. Number density versus chemical potential at $m = 0.1$ for a 6×6 lattice: comparison of CL (blue) and RCL (red) results with phase-quenched reweighting benchmarks (solid).

V. CONCLUSIONS

Previous studies have shown that the complex Langevin method can solve the sign problem occurring in simulations of theories with a complex action, however, caution should be exercised as this requires the CL validity conditions to be satisfied. It turns out that these conditions are often only satisfied for some range of parameters, while they are violated for other parameter values, in which case CL gives wrong results. Herein I introduced the *reweighted complex Langevin* (RCL) method, which combines the CL method with a reweighting of the complex trajectories to enlarge the applicability range of the method. As a proof of principle we presented first results of the method on a one-dimensional partition func-

tion and on two-dimensional strong-coupling QCD and verified that the RCL procedure indeed yields the correct results, even when CL itself does not work for the target ensemble.

Although we herein focussed on cases where CL does not satisfy the validity conditions for the target ensemble, the RCL method can also be applied in cases where CL works fine in the target ensemble with the aim to reuse already existing trajectories obtained at different parameter values and hence gain simulation time. The fact that target and auxiliary ensembles can be chosen close to one another should form a clear advantage over other reweighting methods.

Another possible avenue is to use RCL to interpolate instead of extrapolate in the reweighting parameter, for example the chemical potential in QCD, as we could combine results obtained from auxiliary ensembles at parameter values above and below the target value. This again could improve the quality of the RCL estimates compared to standard reweighting.

The method is of course not constrained to reweighting in a single parameter, and it could be further optimized by making a multiparameter reweighting [14], for example using the chemical potential and quark mass in QCD.

Even so, it is to be expected that the overlap and sign problems will deteriorate the efficiency of RCL, as for any reweighting method, once the auxiliary and target ensembles are too distant. The efficiency of the method and the optimization of reweighting strategies will be studied in more detail in forthcoming work.

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