

Complex Langevin boundary terms in lattice models

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In complex Langevin simulations, the insufficient decay of the probability density near infinity leads to boundary terms that spoil the formal argument for correctness. We present a formulation of this term that is cheaply measurable in lattice models, and in principle allows also the direct estimation of the systematic error of the CL method. Results for a toy model, 3d XY model and HDQCD are presented.

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1. Introduction

The notorious sign problem invalidates importance sampling simulations of theories with a complex measure, e.g. QCD at nonzero chemical potential. A proposed solution to this problem is the complex Langevin method [1] which complexifies the integration manifold using holomorphy, and uses the Complex Langevin equation (CLE), to evade the need of interpreting the integration measure as a probability density. For some complex measure $\rho(x) = \exp(-S(x))$ depending on the variable x the CLE is thus written as

$$\partial_\tau x = -\text{Re} \left. \frac{\partial S(z)}{\partial z} \right|_{z=x+iy} + \eta_\tau, \quad \partial_\tau y = -\text{Im} \left. \frac{\partial S(z)}{\partial z} \right|_{z=x+iy}, \quad (1)$$

with the drift term $K(z) = \partial S(z)/\partial z$ and a Gaussian noise η satisfying $\langle \eta_\tau \eta_{\tau'} \rangle = 2\delta(\tau - \tau')$. This method is successful in many cases [2], (for gauge theories there is an extra difficulty caused by the complexification of gauge degrees of freedom, which is cured by gauge cooling[3]). In some cases however problems remain, leading to convergence to incorrect results. It has been identified that the problematic cases either have to do with insufficiently fast decay of the probability density of the complexified stochastic process at infinity [4] or near zeroes of the measure [5]. In the formal justification of the Complex Langevin method, this gives rise to certain boundary terms invalidating the equivalence of the Complex Langevin result to the correct result, which is simply given by the integral on the original manifold with the complex measure. Here we discuss boundary terms arising at infinity, for boundary terms around poles, see [6].

2. Boundary terms

The CLE gives rise to a real probability density on the complexified manifold $P(x, y, \tau)$. (To keep the notation simple we use a one variable model, generalizations to more variables are straightforward). The CLE result for a holomorphic observable $O(z)$ is thus

$$\langle O \rangle_{P(t)} = \int dx dy P(x, y, t) O(x + iy), \quad (2)$$

whereas the correct result we intend to calculate is

$$\langle O \rangle_\rho = \int dx O(x) \rho(x) = \lim_{t \rightarrow \infty} \langle O \rangle_{\rho(t)} = \lim_{t \rightarrow \infty} \int dx O(x) \rho(x, t) \quad (3)$$

where we defined a time-dependent complex measure $\rho(x, t)$ using $\rho(x, t) = \exp(L_c^T t) \rho_0(x)$, where $\rho_0(x)$ can be some initial distribution on the real axis, and L_c is the complex Fokker-Planck operator $L_c = (\partial_z + K(z)) \partial_z$. Assuming the uniqueness of the limit $\rho(x, t) \rightarrow e^{-S(x)}$, one can define an interpolation function

$$F(t, \tau) = \int dx dy P(x, y, t - \tau) O(x, y, \tau), \quad (4)$$

using the time evolved observables

$$O(x, y, t) = e^{t L_c} O(x + iy). \quad (5)$$

$F(t, \tau)$ interpolates between the above two quantities such that $F(t, 0) = \langle O \rangle_{P(t)}$ and $F(t, t) = \langle O \rangle_{\rho(t)}$, provided the initial conditions are chosen to agree. Thus the CLE results are correct if $\partial F(t, \tau)/\partial \tau = 0$, which can be shown using partial integrations assuming holomorphy of the evolved observables. However the partial integrations can give rise to boundary terms if the decay of $P(x, y)$ is not fast enough at infinity. Introducing a cutoff in the integral we can derive the formula for the boundary term at infinity:

$$B(Y, t) = \partial_\tau F(Y; t, \tau)|_{\tau=0} = \int_{|y| < Y} dx dy \partial_y (K_y O(0) P(x, y, t)) = \int_{y=Y} \mathbf{n} K_y P(t) O(0) dx dS \quad (6)$$

where the integral over a divergence is converted to an integral over a surface with dS the surface element and \mathbf{n} is a normal vector. Using this definition the boundary term for a toy model was measured in [7]. This definition allows the calculation of the boundary term also in models with many independent variables, by defining a cutoff which restricts the variables to a compact subspace which encompasses the whole complexified manifold as the cutoff Y is sent to infinity. However the integration on the surface of such a compact region can be cumbersome for models with many variables. Instead we turn to different formulation of the boundary terms.

Following [8], starting again from $B(Y, t) = \partial_\tau F(Y; t, \tau)$, we write

$$\partial_\tau F(Y; t, \tau)|_{\tau=0} = - \int_{|y| \leq Y} \partial_t P(x, y, t) O dx dy + \int_{|y| \leq Y} P(x, y, t) L_c O dx dy. \quad (7)$$

The first term in this expression goes to zero in the $t \rightarrow \infty$ limit, as the process equilibrates and $P(x, y, t)$ evolves to a stationary solution. The second term can be nonzero and it can spoil correctness if $\lim_{Y \rightarrow \infty} B(Y) \neq 0$. We can similarly define higher order boundary terms using

$$B_n(Y) = \partial_\tau^n F(Y; t, \tau)|_{\tau=0} = \lim_{t \rightarrow \infty} \int_{|y| \leq Y} P(x, y, t) L_c^n O dx dy = \langle \Theta(Y - |y|) L_c^n O \rangle_P. \quad (8)$$

This construction can be straightforwardly generalized to lattice systems with many variables by defining an integration cutoff with e.g. $\max_i y_i < Y$. Generalization to curved manifolds such as the $SL(3, \mathbb{C})$ space arising in the complexification of lattice QCD simulations is e.g. possible using the unitarity norm

$$n(M) = \text{Tr}(M^\dagger M - 1)^2 \text{ for } M \in SL(N, \mathbb{C}). \quad (9)$$

The boundary term is then defined using the Haar measure dM as

$$B_n(Y) = \int_{n(M) < Y} P(M) L_c^n O dM = \langle \Theta(Y - n(M)) L_c^n O \rangle_P. \quad (10)$$

For lattice models one can take $n(M)$ as the average or the maximum of the univarity norms of the link variables.

The boundary term arises in the limit that the cutoff is taken to infinity, as well as the Langevin time. The order of limits is however crucial. As we see above $B(Y = \infty) = 0$ expresses the stationarity of the complexified process, and thus $B(Y = \infty)$ is consistent with zero within errors (large fluctuations give a hint for incorrect CLE results). If we take the $Y \rightarrow \infty$ limit last, the observation of a nonzero boundary term is possible.

3. Results

First we investigate the toy model given by $S(\varphi) = i\beta \cos(\varphi) + s\varphi^2/2$. For $s = 0$, the CLE equilibrates to $P(x, y) = 1/(4\pi \cosh^2 y)$, giving an incorrect value for the observables $e^{ik\varphi}$ with $k \in \mathbb{Z}$ [9]. The second term in the action acts as a regularizer and ensures correct CLE results if s is chosen sufficiently large as can easily be verified using numerical integration. The boundary term is measured using eq. (8), as seen in Fig. 1. As one observes a nonzero $\lim_{Y \rightarrow \infty} B(Y)$ limit signals an incorrect CLE result. Note that in the case of incorrect CLE results, the boundary term's fluctuations grow as Y grows. For the rightmost value on the plot the cutoff is removed, and the value $B(Y)$ is consistent with zero within errors, as argued above. For this toy model, the whole τ

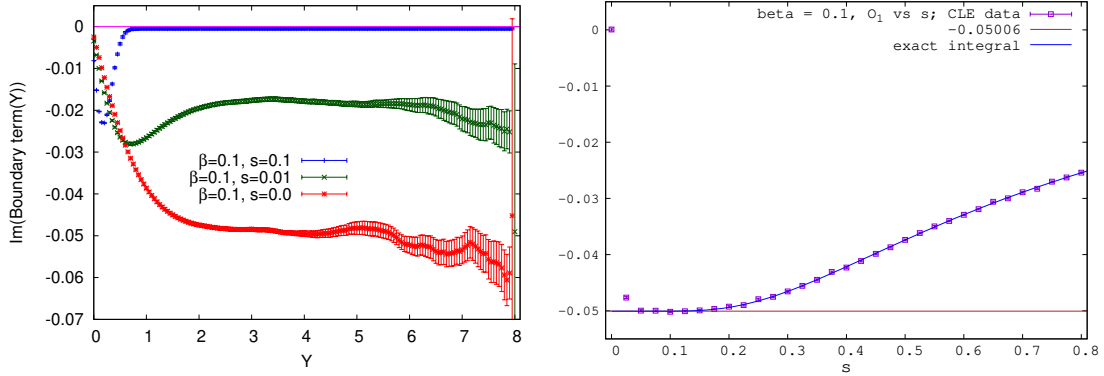


Figure 1: Boundary term for the observable e^{ix} in the toy model $S(\varphi) = i\beta \cos(\varphi) + s\varphi^2/2$, for various s values (left). The average $\langle e^{ix} \rangle$ in the CLE process and its exact value as a function of s for $\beta = 0.1$ (right).

dependence of $F(t, \tau)$ is calculable using the solution of the Fokker-Planck equation for $P(x, y, t)$ and a numerical solution of the differential eqs. defining $O(z, t)$ [7], see in Fig. 2. As one observes,

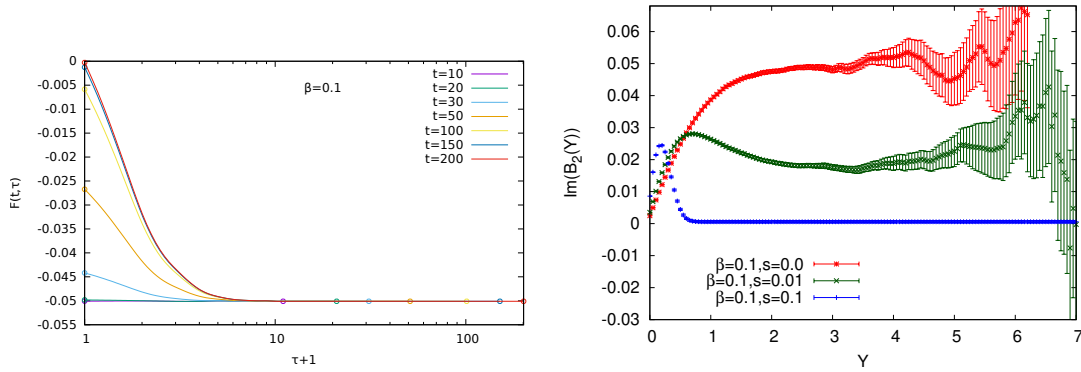


Figure 2: The interpolation function $F(t, \tau)$ for the observable $e^{i\varphi}$ in the toy model $S(\varphi) = i\beta \cos(\varphi) + s\varphi^2/2$, for $\beta = 0.1$ and various t, τ values (left). The second order boundary term B_2 for the observable $e^{i\varphi}$.

the τ dependence of $F(t, \tau)$ can be approximated with an ansatz.

$$F(t, \tau) \approx \sum_{n=0}^{\infty} A_n(t) \exp(-\omega_n \tau) \quad (11)$$

β, s	B_1	B_2	CL	correct	corrected CL
0.1, 0	-0.04859(45)	0.0493(11)	-0.00115(45)	-0.05006	-0.04901(62)
0.1, 0.01	-0.01795(49)	0.01801(80)	-0.03318(50)	-0.05006	-0.05106(40)
0.1, 0.1	-0.00048(30)	0.00057(35)	-0.04957(31)	-0.05006	-0.04997(6)
0.5, 0	-0.2474(11)	0.237(11)	0.00003(23)	-0.25815	-0.258(11)
0.5, 0.3	-0.05309(86)	0.0552(51)	-0.19658(70)	-0.23841	-0.2473(37)

Table 1: The estimation of the correct result using the correction formula (13) for the toy model $S(\varphi) = i\beta \cos(\varphi) + s\varphi^2/2$ the imaginary part of the observable e^{ix} .

To get the error of the CLE solution, we must calculate

$$F(t, 0) - F(t, t) = \langle O \rangle_P - \langle O \rangle_\rho. \quad (12)$$

Using the simplified ansatz $F(t, \tau) = A_0 + A_1 \exp(-\omega_1 \tau)$, we can express the error using the boundary terms:

$$F(t, 0) - F(t, t) = \frac{(\partial_\tau F(t, \tau))^2}{\partial_\tau^2 F(t, \tau)} \Big|_{\tau=0} = \frac{B_1^2}{B_2} \quad (13)$$

This allows to calculate a corrected result with $\langle O \rangle_{\text{corr}} = \langle O \rangle_P - B_1^2/B_2$. On Fig. 2 the second order boundary term is plotted. Compared to B_1 they have larger fluctuations so large statistics is needed for a reliable measurement. As shown in Table. 1 this allows the recovery of the correct result within errors.

We have studied the boundary terms in the 3D XY model

$$S = -\beta \sum_x \sum_{\nu=0}^2 \cos(\phi_x - \phi_{x+\hat{\nu}} - i\mu\delta_{\nu,0}) \quad (14)$$

for which the CLE is known to fail in the small β phase even for small chemical potentials, and is apparently correct in the large β region [10]. The measurement of the boundary terms confirms this picture, see in Fig. 3. Apparently a boundary term is present even at $\beta = 0.9$, but its value is so small, that for all intents and purposes the CLE gives correct results. The correction of the observables using eq. 13 gives the right magnitude and sign of the systematic error of CLE, however the exact result (calculated using the worldline method) in the low beta phase is not recovered. The reasons for this might include the simplicity of the ansatz for $F(t, \tau)$ as well as the difficulty of the measurement of the second order boundary terms due to lack of necessary statistics (For further details, see [8]).

Finally we show results for the HDQCD model [11]. As noted in [3] the CLE treatment gives correct results for large β values, and incorrect result below $\beta \approx 5.8$. The measurement of the boundary terms confirms this picture. In Fig. 4 the boundary term for the spatial plaquette and the Polyakov loop variable is shown. In Fig. 5 CLE results and reweighting results are shown, confirming that it is possible to judge the reliability of CLE results based on the boundary terms.

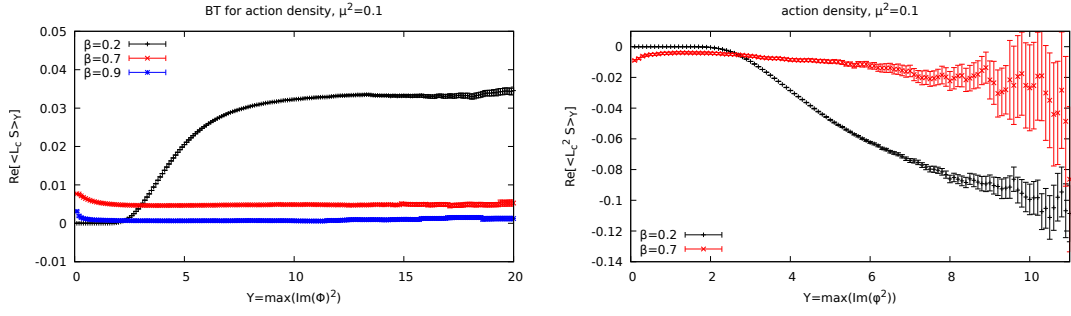


Figure 3: The first order (left) and second order (right) boundary term in the 3D XY model for the action density observable.

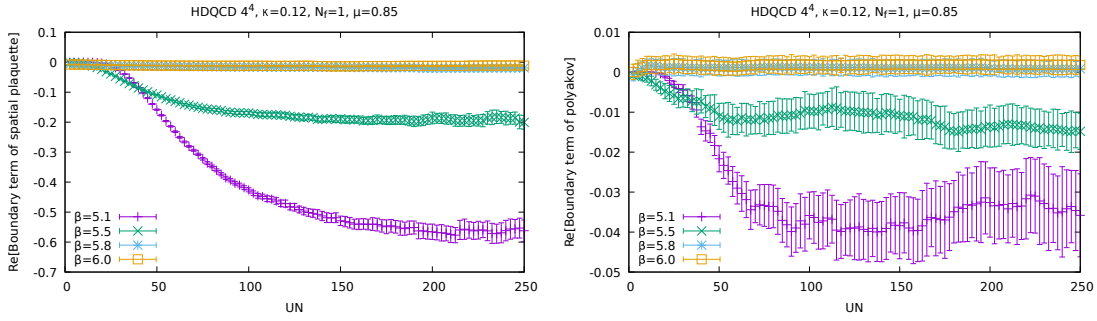


Figure 4: The boundary term in HDQCD for the spatial plaquette average observable (left) and the Polyakov loop observable (right).

4. Conclusions

We have shown that the boundary terms present a valuable diagnostic tool for the assessing of the performance of a CLE simulation. In the volume integral formulation, they can be measured as the limiting value of a cut-off version of the observable $L_c O$ for the observable O . The boundary term observables are cheap to measure even for lattice models, and one needs a cheap offline analysis procedure to calculate the dependence on the cutoff. The order of magnitude of the systematic error of CLE is then related to the magnitude of the boundary terms. In some cases even the correction of the CLE result can be carried out using second order boundary terms.

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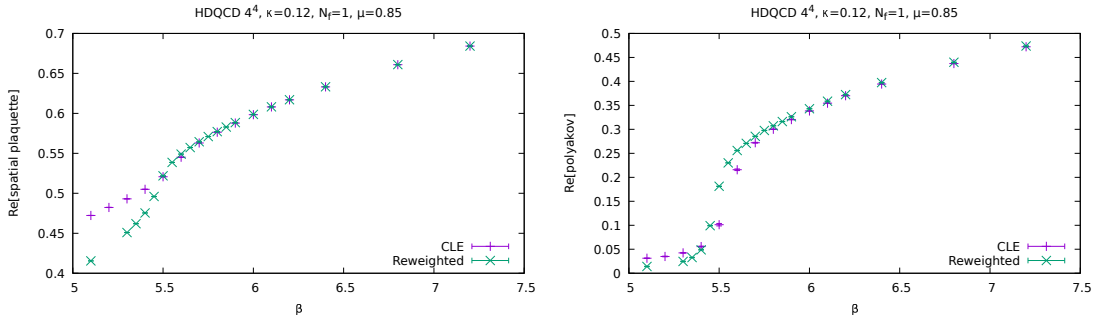


Figure 5: Comparing reweighting and CLE results in HDQCD: spatial plaquette (left) and Polyakov loop average (right).

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