PROCEEDINGS OF SCIENCE

Complex Langevin: Boundary terms at poles of the drift

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The complex Langevin method is a general method to treat systems with complex action, such as QCD at nonzero density. The formal justification relies on the absence of certain boundary terms, both at infinity and at the unavoidable poles of the drift force. Here I focus on the boundary terms at these poles for simple models, which so far have not been discussed in detail. The main result is that those boundary terms (for the "un-evolved" observables) arise after running the Langevin process for a finite time and vanish again as the Langevin time goes to infinity. This is in contrast to the boundary terms at infinity, which can be found to occur in the long time limit (cf. the contribution by Dénes Sexty).

The 38th International Symposium on Lattice Field Theory, LATTICE2021 26th-30th July, 2021 Zoom/Gather@Massachusetts Institute of Technology

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PoS(LATTICE2021)210

1. Introduction

This contribution is based largely on [1], to which we refer for more details.

To be able use stochastic sampling methods for a complex holomorphic density $\rho \propto e^{-S}$ on $\mathbb{R}^d$, one searches for a probability density $P \geq 0$ on $\mathbb{C}^d$, s.t.

$$\langle O \rangle \equiv \int_{\mathbb{R}^d} O(x)\rho(x)dx = \int_{\mathbb{C}^d} O(x+iy)P(x,y)dxdy\,. \tag{1}$$

for *holomorphic* observables O.

Klauder [2] and Parisi [3] proposed a general, very flexible method to produce such a P, as the equilibrium distribution of *real stochastic process* on $\mathbb{C}^d$, called *Complex Langevin* (CL) method, by defining

$$dz = Kdt + dw, \quad K = -\nabla S \tag{2}$$

(dw is the real Wiener increment normalized as $\langle dw^2 \rangle = 2$). This process necessarily wanders into the complex realm $\mathbb{C}^d$. Written out (2) becomes

$$dx = K_x dt + dw, \quad K_x = \mathrm{Re}\, K \tag{3}$$

$$dy = K_y dt, \quad K_y = \mathrm{Im}\, K \tag{4}$$

The hope is then that the long time average of this process yields the ρ-expectation. A strategy to justify this was proposed in [4]. Briefly it proceeds as follows: we want for a sufficiently large class of observables O

$$\langle O \rangle_{\rho(t)} = \langle O \rangle_{P(t)} \quad \forall\, t \geq 0\,, \tag{5}$$

where $P(t) \equiv P(x,y;t)$ is the probability density of the CL stochastic process and $\rho(t) \equiv \rho(x;t)$ is the evolved complex density solving the “complex Fokker-Planck equation”

$$\frac{\partial}{\partial t}\rho(z;t) = L_c^T \rho(z;t)\,, \quad L_c^T = \partial_z(\partial_z - K(z))\,. \tag{6}$$

with initial conditions such that (5) holds at $t=0$. L_c^T is the transpose of L_c, governing the evolution of observables:

$$\frac{\partial}{\partial t} O(z;t) = L_c O(z;t)\,, \quad L_c = (\partial_z + K(z))\partial_z\,. \tag{7}$$

It is easy to see that

$$\int dx \rho(x;t) O(x;0) = \int dx \rho(x;0) O(x;t) \tag{8}$$

provided the integration connects two zeroes (finite or infinite) of ρ. Eq.(5) is then true if the function

$$F_O(t,\tau) \equiv \int P(x,y;t-\tau) O(x+iy;\tau) dx\, dy \quad (0 \leq \tau \leq t) \tag{9}$$

is independent of τ, i.e.

$$\frac{\partial}{\partial \tau} F_O(t,\tau) = 0 \quad \forall t \geq 0\,. \tag{10}$$

Here $O(z;\tau)$ is the solution of the initial value problem

$$\frac{\partial}{\partial \tau} O(z;\tau) = L_c O(z;\tau)\,, \quad O(z;0) = O(z)\,; \quad L_c = (\partial_z + K(z))\partial_z\,, \tag{11}$$

(5) follows from (10) because $F_O(t,\tau)$ interpolates between two sides of (5), as shown in [4] (assuming integration by parts in x without boundary terms). Integration by parts in x, y shows that (10) holds, up to possible boundary terms, in other words $\frac{\partial}{\partial\tau}F(t,\tau)$ **is** a (sum of) boundary terms. Boundary terms may arise at infinity as well as at poles.

An important caveat that was stated in [4] is the following: (5) implies correctness of CL only if

$$\lim_{t\to\infty}\langle O\rangle_{\rho(t)} \tag{12}$$

exists and is unique. i. e. if the spectrum of L_c^T lies in the left half of $\mathbb{C}$ and 0 is a simple eigenvalue with eigenfunction $\rho(x)$ (see the remark at the end of Section 3).

Possible failure of the CL method was analyzed from a different point of view by Salcedo [5]; the problem caused by poles of the drift was studied by Nishimura and Shimasaki in simple models [6]; in [7] we presented a detailed study of this issue, with the emphasis on numerical analysis of various models, from the simplest one-dimensional case to full QCD. Here we trace the problem to the occurrence of boundary terms.

2. The need to consider the evolution before reaching equilibrium

In [8, 9] we found boundary terms at infinity by considering the equilibrium distributions and "un-evolved" observables, i. e. $\partial_\tau F(t,\tau)|_{\tau=0}$ (cf. D. Sexty, these proceedings).

But this type of boundary term does not appear at poles. This is because empirically the equilibrium distribution $P(x,y;t=\infty)$ vanishes at least linearly at the poles of the drift, so holomorphic observables could not lead to boundary terms there. (Note that this argument does not hold for "evolved" observables, which are at best meromorphic.)

To see this in a little more detail, let's consider for simplicity a pole at the origin; consider the approximate boundary term

$$\int_{x^2+y^2\le\delta^2} dx\,dy P(x,y;t=\infty)L_cO(x+iy)\,. \tag{13}$$

Using the Cauchy-Riemann equations and integrating by parts (13) becomes

$$\int_{x^2+y^2\le\delta^2} dx\,dy O(x+iy)(L^TP)(x,y;t=\infty)+B_\delta=B_\delta \tag{14}$$

where L^T is the *real* Fokker-Planck operator

$$L^T=\partial_x^2-\partial_xK_x-\partial_yK_y \tag{15}$$

describing the evolution of P under the stochastic process, see [4]). (14) holds since the first term of the left-hand side vanishes in equilibrium. B_δ is a boundary term. Now, since O is holomorphic, L_cO has at most a simple pole at the origin, stemming from the pole in the drift. Since P vanishes linearly at the origin, the integrand of (13) is bounded in the region of integration, hence the boundary term vanishes for $\delta\to 0$.

If instead we consider the time evolution for finite time t, B_δ now is given by

$$B_\delta=\int_{x^2+y^2\le\delta^2} dx\,dy\,\left\{O(x+iy)L^TP_{z_0}(x,y;t)-P_{z_0}(x,y;t)L_cO(x+iy)\right\} \tag{16}$$

and the first term of this expression is no longer zero. Since the equilibrium distribution does not lead to a boundary term, we now consider the evolution for short times.

3. One-pole model

The one-pole model is defined by

$$\rho(x) = (x - z_p)^{n_p} \exp(-\beta x^2) \tag{17}$$

with n_p a positive integer.

Since we are not interested in large times, we can simplify the model even further by putting $\beta = 0$, giving rise to the "pure pole model"; without loss we also set $z_p = 0$. For the special case $n_p = 2$ there is an explicit formula for the integral kernel of $\exp(tL_c)$:

$$\exp(tL_c)(z,z') = \frac{z'}{z\sqrt{4\pi t}} \exp\left(\frac{(z-z')^2}{4t}\right), \tag{18}$$

where $z' = x' + iy_0$ and the integration is over x'. As observables we take the powers

$$O_k(z) \equiv z^k\,, k = -1, 0, 1, 2 \ldots . \tag{19}$$

Using (18) we can explicitly compute the evolution of those observables, obtaining e. g.

$$\begin{aligned}
O_{-1}(z;t) &= \frac{1}{z}\,. \\
O_1(z;t) &= z + \frac{2t}{z}\,, \\
O_2(z;t) &= z^2 + 6t\,, \\
O_3(z;t) &= z^3 + 12tz + \frac{12t^2}{z}\,, \\
O_4(z;t) &= z^4 + 20tz^2 + 60t^2\,,
\end{aligned} \tag{20}$$

The fact that no higher negative powers occur for $n_p =$ was already noted in [7]. We compared these results with those of the CL evolution $\langle O_k \rangle_{P(t)}$ obtained by running 10^5 CL trajectories, all with the same starting point $z = z_0$ up to the desired time t. The comparison is shown in Fig. 1 for $k = -1$ and $k = 4$.

As in these examples, generally for even powers there is agreement, whereas for odd powers already at small times there is disagreement, signaling the presence of boundary terms for these powers.

As long as $n_p = 2$ we also have a closed expression for the integral kernel $\exp(tL_c)$ for $\beta > 0\,, z_p = 0\,, n_p = 2$:

$$\begin{aligned}
\exp(tL_c)(z,z') =& \frac{z'}{z} \exp\left(\frac{\beta}{2}(z^2 - z'^2)\right) \exp(2\beta t) \\
&\times \sqrt{\frac{\beta}{\pi(1-e^{-4\beta t})}} \exp\left[-\frac{\beta(z^2+z'^2)}{2\tanh(2\beta t)}\right] \exp\left(\frac{\beta z z'}{\sinh(2\beta t)}\right)
\end{aligned} \tag{21}$$

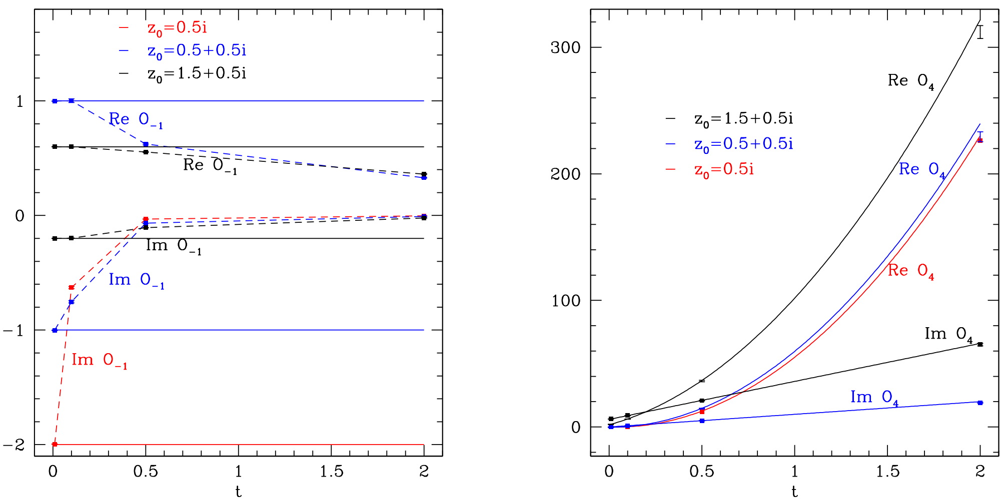

Figure 1: Pure pole model. Comparison of two evolutions for $k = -1$ (left) and $k = 4$ (right). Dashed lines: connecting CL results, solid lines: analytic ρ evolution (20).

(based on Mehler's formula [10]). Here again $z' = x' + y_0$, x' being the integration variable.

Defining

$$b \equiv \frac{\beta}{\sinh(2\beta t)}\,; \qquad \sigma \equiv \frac{1-\exp(-4\beta t)}{2\beta}\,, \tag{22}$$

we find for the same observables as above

$$\begin{aligned}
O_2(z;t) &= 3\sigma + b^2\sigma^2 z^2 \to \frac{3}{2\beta} \quad (t\to\infty)\\
O_4(z;t) &= 15\sigma^2 + 10b^2\sigma^3 z^2 + b^4\sigma^4 z^4 \to \frac{15}{4\beta^2} \quad (t\to\infty)\\
O_1(z;t) &= \frac{1}{bz} + b\sigma \to \infty \quad (t\to\infty)\\
O_3(z;t) &= \frac{3\sigma}{bz} + 6b\sigma^2 z + b^3\sigma^3 z^3 \to \infty \quad (t\to\infty)\\
O_{-1}(z;t) &= \frac{1}{b\sigma z} \to \infty \quad (t\to\infty)
\end{aligned} \tag{23}$$

Even powers remain bounded for $t \to \infty$ and actually converge to the correct limit, whereas odd powers grow exponentially!

This signals the presence of an exponentially growing mode in both $\exp(tL_c)$ and its transpose $\exp(tL_c^T)$, so in this case $\langle O\rangle_{\rho(t)}$ is *not* the correct evolution. This failure of correctness is again due to the existence of boundary terms: absence of boundary terms also implies absence of exponentially growing modes as will be demonstrated elsewhere [11].

4. Direct numerical evaluation of the boundary term

We now consider $\beta > 0, z_P \neq 0$. In this case we do not have an analytic expression for the integral kernel of $\exp(ptL_c)$, but we can numerically evaluate the approximate boundary term B_δ (16).

After some easy manipulations we find for *any* holomorphic observable $O(z)$

$$B_\delta = -\oint_{|z-z_p|=\delta} \vec{K}\cdot\vec{n}\, P_{z_0}(x,y;t)O(x+iy)ds + o(\delta) = -\oint_{|z-z_p|=\delta} \vec{K}\cdot\vec{n}P_{z_0}(x,y;t)O(0)ds + o(\delta)\,, \tag{24}$$

We approximate the circle of radius δ in (24) by a thin ring of thickness $\eta\delta$:

$$(1-\eta)\delta < |z - z_p| < (1+\eta)\delta\,. \tag{25}$$

For $n_p = 2, \beta = 1, z_p = -i/2, z_0 = i/2$ and $O(0) = 1$ the CL process gives the results shown in Fig. 2.

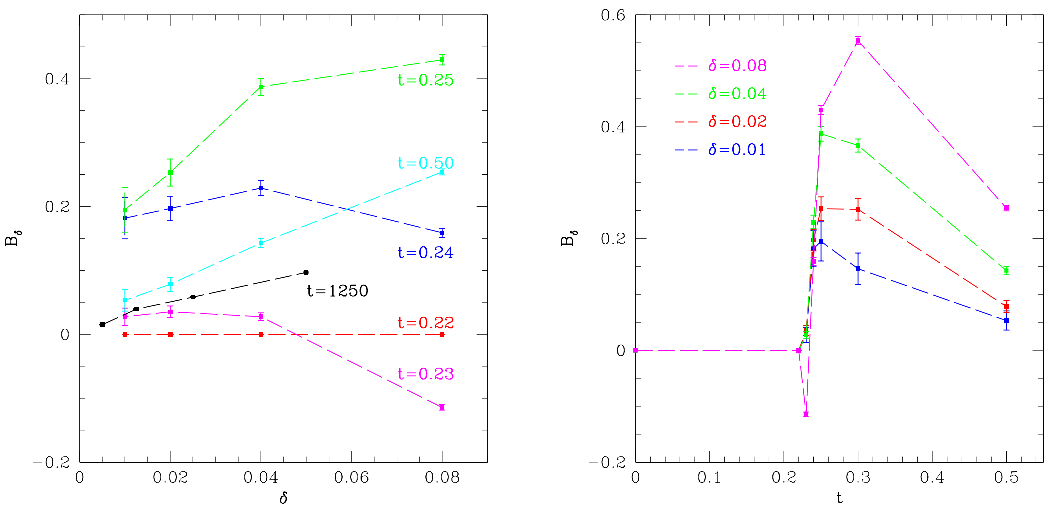

Figure 2: Full pole model. Numerical estimates of the boundary term B_δ for $\eta = 0.1$. Left: B_δ vs. δ, right: B_δ vs. t.

The CL data are produced as before by running trajectories up to the respective times t. Because the chance of hitting the small rings is so small, we took here 10^7 trajectories, but we still obtained only about 50 hits for $\delta = 0.01$, $\eta = 0.1$ and $t = 0.24$ and 0.25, and even fewer for other values of t. Therefore the extrapolation to $\delta = 0$ can only be to be done “by eye”. But Fig. 2 still shows clearly that for $t < 0.22$ there is no boundary term. This is because the process takes at least that much time to move from the starting point to the location of the pole. (Because there is no noise in the y direction one can compute this time by evaluating a simple integral.)

For $0.23 < t \leq 0.25$ there are clear indications of a boundary term, whereas for $t > 0.5$ it is fading away, and it has disappeared for $t = 1250$, where we get much smaller statistical errors because we can thermalize and average over initial conditions.

But it should be stressed that we were considering $\partial_\tau F(t,\tau)$ only for $\tau = 0$. It is to be expected that for $t > 0.5$ the boundary term reappears at nonzero values of τ.

I would like to thank all the people with whom I had the pleasure of collaborating on the CL method: Gert Aarts, Felipe Attanasio, Lorenzo Bongiovanni, Pietro Giudice, Benjamin Jäger, Frank James, Jan Pawlowski, Lorenzo Luis Salcedo, Manuel Scherzer, Dénes Sexty, Ion-Olimpiu Stamatescu, Jacek Wosiek.

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