Complex Langevin: Boundary Terms at Poles

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1. Complex Langevin

To sample complex holomorphic density $\rho \propto e^{-S}$ on $\mathbb{R}^d$

search for

$P \geq 0$: probability density on $\mathbb{C}^d$, s.t.

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

for holomorphic observables $\mathcal{O}$.

Klauder, Parisi 1983:
P equilibrium distribution of real stochastic process on $\mathbb{C}^d$.

$K = -\nabla S$ complex:

$$dz = K dt + dw, \quad K = -\nabla S$$

($dw \propto$ real Wiener increment $dw = \eta(t) dt$, η white noise).
Process wanders into the complex realm $\mathbb{C}^d$

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

$$dy = K_y dt, \qquad K_y = \mathrm{Im}\, K$$

ρ holomorphic $\Longrightarrow K$ meromorphic

Zeroes of ρ produce poles of K!

2. Boundary terms may cause problems

(Aarts, ES, Sexty, Stamatescu: PRD81(2010) 054508)

Want:

$$\boxed{\langle \mathcal{O} \rangle_{\rho(t)} = \langle \mathcal{O} \rangle_{P(t)} \quad \forall\, t \geq 0} \; (*)$$

true if

$$\frac{\partial}{\partial \tau} F(t,\tau) = 0 \quad \text{(boundary term)}$$

and $(*)$ holds for $t = 0$
where

$$F(t,\tau) \equiv \int P(x,y;t-\tau)\mathcal{O}(x+iy;\tau)dx\,dy$$

interpolates between two sides of $(*)$.

Boundary terms from integration by parts

- at ∞

-at poles

Evolution of observables

$\mathcal{O}(z)$ holomorphic, $K(z)$ at least meromorphic:

$$\partial_t \mathcal{O}(z;t) = L_c \mathcal{O}(z;t)\,, \quad L_c \equiv [\nabla_z + K] \cdot \nabla_z\,;$$

$$\mathcal{O}(z;0) = \mathcal{O}(z)$$

Expect: $\mathcal{O}(z;t)$ meromorphic where K is.

Duality:

$$\boxed{\langle \mathcal{O} \rangle_{\rho(t)} = \mathcal{O}(x_0 + iy_0; t)}$$

(integration by parts, need $\rho \to 0$ for $|x| \to \infty$)

3. No boundary term at pole for $t = \infty$

Previous talk by D. Sexty: Boundary terms at ∞ found at $t = \infty$.

At pole of K: $P_{\mathrm{eq}} = \lim_{t\to\infty} P(x, y; t)$ vanishes linearly.

Pole at 0. Look at

$$B_\delta \equiv \int_{x^2+y^2\leq\delta^2} dx\, dy P_{\mathrm{eq}}(x, y) L_c \mathcal{O}(x + iy) \quad (*).$$

Use Cauchy-Riemann equations, integrate by parts: B_δ is pure boundary term because

$$L^T P_{\mathrm{eq}} = 0$$

$\mathcal{O}$ holomorphic $\Longrightarrow$ integrand of $(*)$ bounded near 0 $\Longrightarrow$ $B_\delta \to 0$ as $\delta \to 0$.

4. Exemplary case: One-pole model

$$\rho(z) = (z - z_p)^{n_p} \exp(-\beta z^2),$$

"Pure pole model": $z_p = 0\,, \beta = 0$

For $n_p = 2$ integral kernel:

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

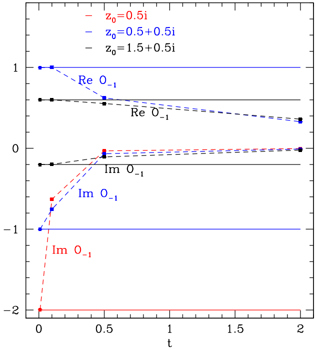
$z' = x' + iy_0$, integrate over x'.

Exact evolution of observables

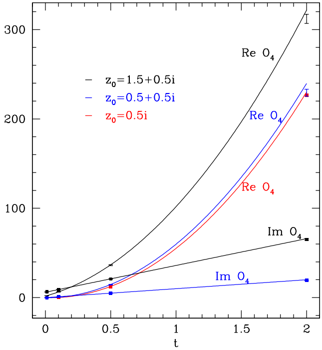
Observables:
$\mathcal{O}_k(z) \equiv z^k, k = 1, \ldots 4$ and $k = -1$.

$$
\begin{aligned}
\mathcal{O}_1(z;t) &= z + \frac{2t}{z}\,, \\
\mathcal{O}_2(z;t) &= z^2 + 6t\,, \\
\mathcal{O}_3(z;t) &= z^3 + 12tz + \frac{12t^2}{z}\,, \\
\mathcal{O}_4(z;t) &= z^4 + 20tz^2 + 60t^2\,, \\
\mathcal{O}_{-1}(z;t) &= \frac{1}{z}\,.
\end{aligned}
$$

Comparison CL – exact evolution



$\mathcal{O}_{-1}$



$\mathcal{O}_4$

odd powers disagree

$\exists$ boundary term

even powers agree

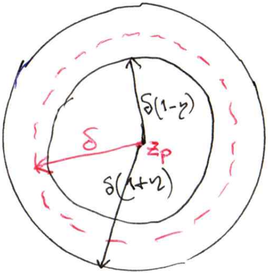
$\nexists$ boundary term

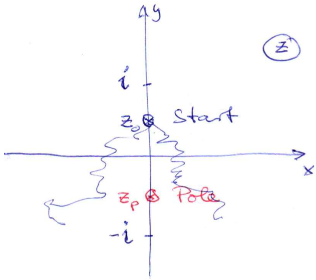
5. Direct evaluation of boundary term

Now $\beta > 0$, $z_p \neq 0$. Approximate boundary term:

$$B_\delta = -\oint_{x^2+y^2=\delta^2} \vec{K} \cdot \vec{n}\, P_{z_0}(x, y; t)\mathcal{O}(x + iy)ds + o(\delta)\,,$$

Approximate circle by rings $(1-\eta)\delta < |z - z_p| < (1+\eta)\delta$





Numerical results:

Choose

$n_p = 2, \beta = 1.0,\ z_p = -0.5\, i,\ z_0 = 0.5\, i$

For these parameters: pole at edge of *supp* $P_{\rm eq} \Longrightarrow$ CL wrong

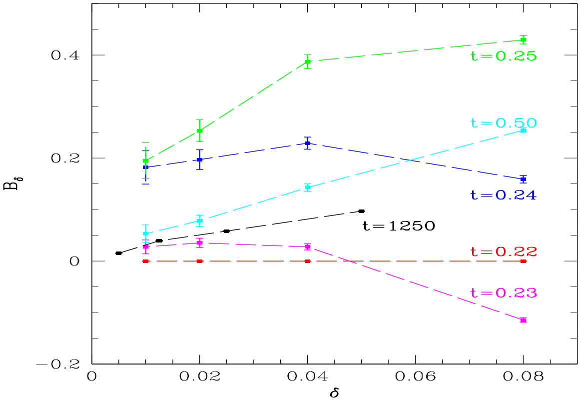
For β large enough, pole outside *supp* $P_{\rm eq} \Longrightarrow$ CL right

(Aarts, Sexty, ES, Stamatescu: JHEP 05 (2017) 044)

Remark:

CL always =
linear combination of integrals over paths between zeroes of ρ.

(conjectured: Salcedo: Phys.Lett. B305 (1993) 125,
proven: Salcedo&ES: J.Phys.A 52 (2019) 3, 035201)



Boundary term arises for $t > 0.23$, disappears for $t \to \infty$.

6. Take-home message:

- Boundary terms at poles are seen at finite Langevin time.

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- Boundary terms at poles are seen at finite Langevin time.
- Boundary terms at ∞ seen at infinite Langevin time.

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