Approaching the sign problem by complexification

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Cold Quantum Coffee

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Contents

The path integral measure and probability

Euclidean path integral

$$Z = \int \mathcal{D}\phi e^{-S(\phi)}$$

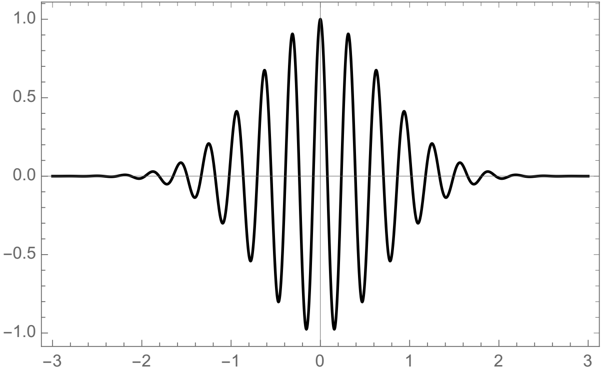
$\rho(\phi) = e^{-S(\phi)}$ is positive $\rightarrow$ probability measure.

Observables via Monte Carlo simulations

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{O} e^{-S}$$

What is the sign problem?

What if $\rho(\phi) = e^{-S(\phi)} \ngtr 0$? Nontrivial cancellations $\to$ high statistics for the tail. (1005.0539)



Or even $\rho(\phi) \in \mathbb{C}$? $\to$ **no Monte Carlo**.

Reweighting

Reweighting (not limited to this particular form):

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{O}\rho}{\int \rho} = \frac{\int \mathcal{O}\mathrm{Arg}\,(\rho)\,|\rho|}{\int \mathrm{Arg}\,(\rho)\,|\rho|} = \frac{\langle \mathcal{O}\mathrm{Arg}\,(\rho)\rangle_{|\rho|}}{\langle \mathrm{Arg}\,(\rho)\rangle_{|\rho|}}$$

denominator:

$$\langle \mathrm{Arg}(\rho)\rangle_{|\rho|} = \left\langle \frac{\rho}{|\rho|} \right\rangle_{|\rho|} = \frac{\int \frac{\rho}{|\rho|}|\rho|}{\int |\rho|} = \frac{Z_\rho}{Z_{|\rho|}}$$

free energy density: $f = -\frac{T}{V}\log Z$:

$$\frac{Z_\rho}{Z_{|\rho|}} = e^{-\frac{V}{T}\Delta f} \xrightarrow{V\to\infty} 0$$

Overlap problem: Strong shift of $\rho \to |\rho|$ can lead to strong suppression of signal of observable.

Who cares?

Interesting Physics!

- Finite density (most famous: QCD phase diagram)
- Real time evolution
- And much more in and beyond QFT!

What now?

Different ideas are needed!

- For QCD Phase diagram: Taylor expansion, continuation from imaginary chemical potential
- Complex Langevin
- Lefschetz Thimbles and other path deformations
- Dual formulations
- Density of states
- ...

Complex Langevin

Langevin

Stochastic process

$$dx = -\frac{\partial S}{\partial x} dt + dw$$

The corresponding Fokker-Planck equation

$$\frac{\partial}{\partial t} \rho(x) = \left[\partial_x \left(\partial_x + \left(\partial_x S(x)\right)\right)\right] \rho(x)$$

has solution

$$\rho(x; t \to \infty) = e^{-S(x)}$$

Complex Langevin

Complexify the field variable (Parisi '83, or see 0807.1597)

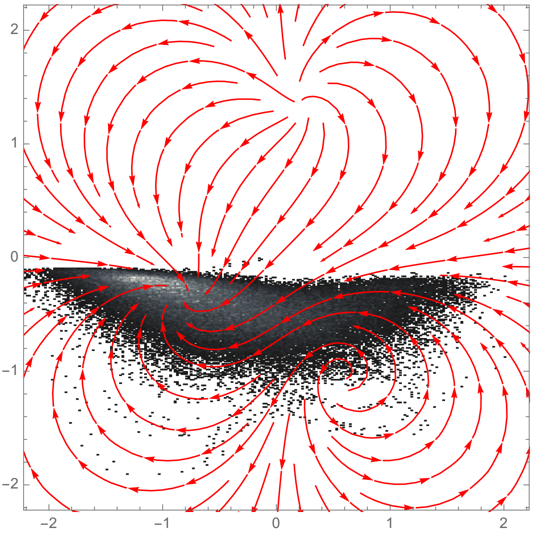
$$dz = -\frac{\partial S}{\partial z} dt + dw$$

or

$$dx = -\mathrm{Re}\left(\frac{\partial S}{\partial z}\right) dt + dw$$
$$dy = -\mathrm{Im}\left(\frac{\partial S}{\partial z}\right) dt$$

What happens?

Langevin evolution is driven by fixpoint structure



When does it work?

Action $S(z)$ (and observables $\mathcal{O}$) holomorphic

Fokker-Planck equation for complex variable and for real and imaginary part, i.e. $\rho(z;t)$ and $P(x,y;t)$

CLE is correct, if: (0912.3360)

$$\langle \mathcal{O} \rangle_{\rho(z;t)} = \langle \mathcal{O} \rangle_{P(x,y;t)}$$

for all t!

When does it work?

Define interpolating quantity

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

with

$$F(t,0) = \langle \mathcal{O} \rangle_{P(x,y;t)}$$
$$F(t,t) = \langle \mathcal{O} \rangle_{\rho(z;t)}$$

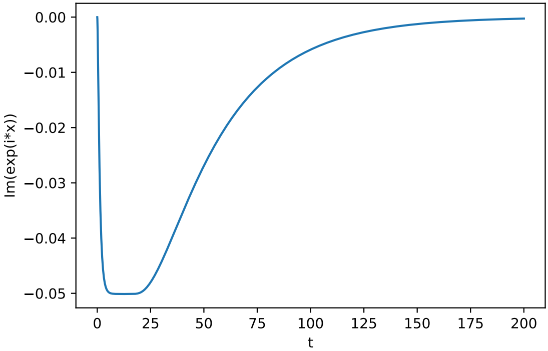
Requirement: $\partial_\tau F(t,\tau) = 0$ (this is true if boundary terms vanish).

Example

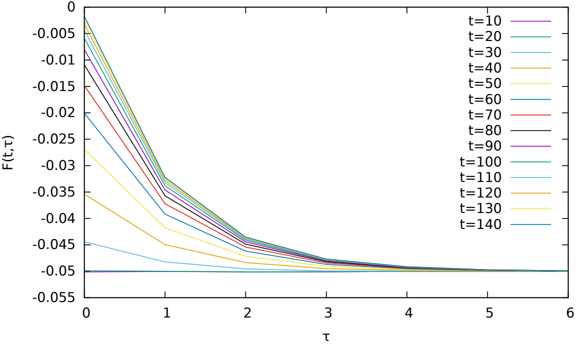
$U(1)$-one link model

$$S(z) = i\beta \cos(z)$$
$$\mathcal{O}(z) = e^{iz}$$

Can be solved numerically (e.g. $\beta = 0.1$):
$\langle \mathcal{O} \rangle = -0.0500626i$. CLE yields: $\langle \mathcal{O} \rangle = 0$. WHY?

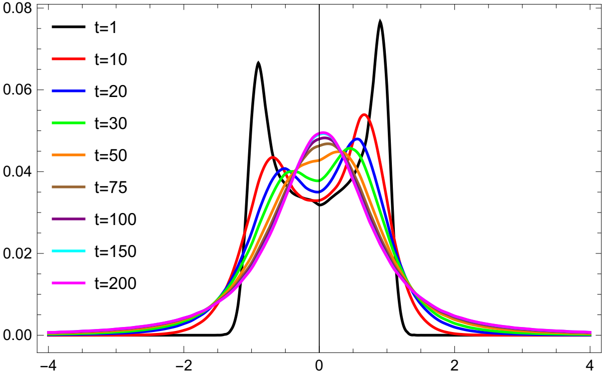


Example



$F(t, \tau)$ shows buildup of boundary effects.

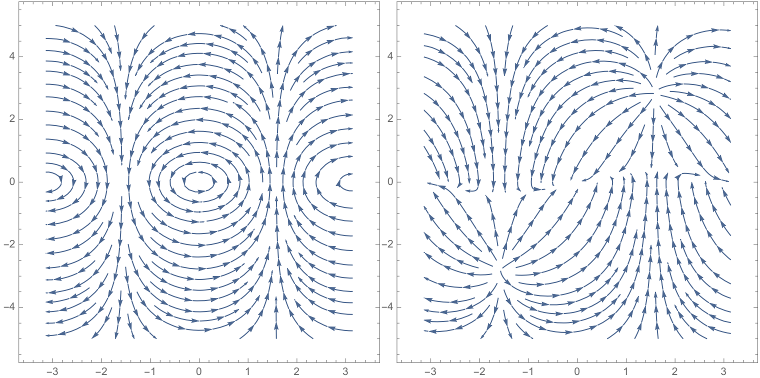
Example



Boundary terms also visible in distribution (only in y-direction, becomes x-independent at large t for this model).

Example

Why does it go wrong? Add term that makes real axis more attractive:



Lack of stable fixed points leads to large excursions.

Summary pt 1/3

There are clear criteria for correctness of CLE!

More complicated theories: Look at histogram of observables instead of solution of Fokker-Planck

$\rightarrow$ one can see if CL is correct by just looking at the simulation results!

Lefschetz Thimbles

The Lefschetz Thimble Method

Look at integrals of the form $Z = \int e^{-s}$

Starting point: Complexification of the real manifold

Find critical points $\frac{\partial S(z)}{\partial z} = 0$

Find Lefschetz thimbles: Steepest descent (ascent) paths that end (start) in the fixpoint

$$\dot{z} = \pm \overline{\frac{\partial S}{\partial z}}$$

Can show: $Im(S)$ is constant along thimbles

The Lefschetz Thimble Method

The following identity holds (1001.2933)

$$\int_{\mathbb{R}} e^{-S(x)} dx = \sum_{\sigma} n_\sigma e^{-Im(S(z_\sigma))} \int_{J_\sigma} e^{-Re(S(z))} dz$$

n_σ is the intersection number of the antithimble (steepest ascent path) with the original manifold, encodes topology

Why does this work? Homotopy-equivalence of the original manifold with the union of (contributing) Lefschetz-thimbles

The Lefschetz Thimble Method

Real weight

$$\rho_\sigma(z) = e^{-Re(S(z))}$$

allows standard Monte Carlo sampling (1205.3996)

$$\langle \mathcal{O} \rangle = \frac{\sum_\sigma n_\sigma e^{-iIm(S(z_\sigma))} Z_\sigma \langle \mathcal{O} \rangle_\sigma}{\sum_\sigma n_\sigma e^{-iIm(S(z_\sigma))} Z_\sigma}$$

$\langle \mathcal{O} \rangle_\sigma$ contains a residual sign problem, due to Jacobian, use reweighting (eq for one thimble:)

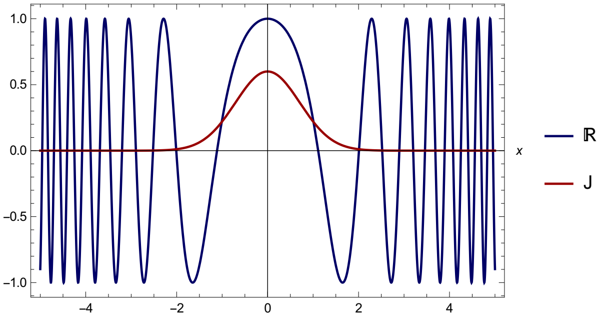
$$\langle \mathcal{O} \rangle = \frac{\langle \mathcal{O} J \rangle}{\langle J \rangle}$$

ratio of weights via reweighting (1803.08418)

$$\frac{Z_1}{Z_2} = \left\langle e^{Re(S_2 - S_1)} \right\rangle_2$$

Why does this help?

Airy integral $S(x) = -i\left(\frac{x^3}{3} + \alpha x\right)$



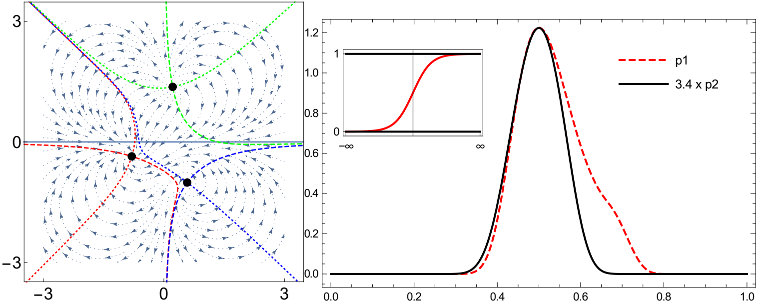
Makes Monte Carlo possible AND removes fluctuations

note: plot borrowed from Felix Zieglers group meeting talk

BUT: Residual sign problem due to Jacobian

Example

$$S(z) = \frac{1}{2}z^2 + \frac{1}{4}z^4 + (1+i)z$$



$$\langle z^2 \rangle_{exact} = 0.73922 + 0.63009i$$

$$\langle z^2 \rangle_{numerical} = 0.73922(6) + 0.63006(4)i \ (1803.08418)$$

Summary pt 2/3

Systematic way to apply Lefschetz Thimble Method in simple systems

We are currently working on field theories

Beyond Lefschetz Thimbles

Using homotopy equivalence, other paths are possible

Maryland approach: Use steepest descent to flow closer to thimbles

Path optimization: Maximize average sign by making an ansatz for a manifold and optimizing the parameters (either by gradient equations or neural networks)

QCD

Complex Langevin and QCD

We look at QCD (first CLE application: 1307.7748)

Lattice action

$$S(U) = -\beta \sum_{n\in\Lambda} \sum_{\mu<\nu} \left(\frac{1}{6} \left[\mathrm{Tr} U_{\mu\nu}(n) + \mathrm{Tr} U_{\mu\nu}^{-1}(n) \right] - 1 \right)$$

$$+ \sum_{\text{flavours}} a^4 \sum_{n,m\in\Lambda} \overline{\psi}(n) D(n|m) \psi(m)$$

$$D(n|m) = \delta_{a,b}\delta_{\alpha,\beta}\delta_{n,m} - \kappa \sum_{\mu=\pm1}^{\pm4} (1-\gamma_\mu)_{\alpha\beta} U_\mu(n)_{ab} \delta_{n+\hat{\mu},m}$$

with $\beta \sim g^{-2}$ and $\kappa \sim 1/m$

Complex Langevin and QCD

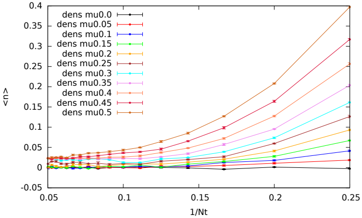
$N_f = 2$ Wilson fermions ($m_\pi \sim 1$GeV so far)

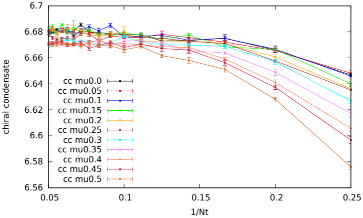
Adaptive stepsize (no runaways)

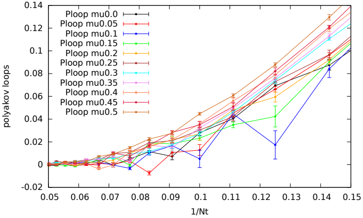
Gauge cooling: keep unitarity norm $N_U = U^\dagger U - Tr1$ as small as possible (gauge transformation opposite to ∇N_U)

Some results

DISCLAIMER: All plots preliminary and low statistics!
$N_s = 8$, $\kappa = 0.15$, $\beta = 5.9$, everything in lattice units
(sorry Nicolas...)

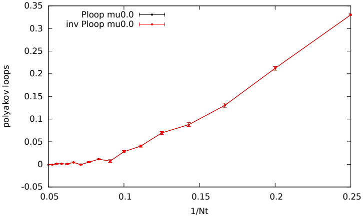


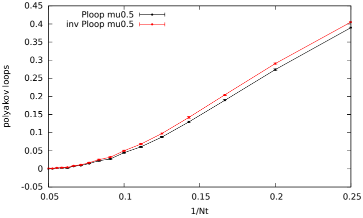




Some results

Debunking CLE = phase quenched





Summary pt 3/3

Sign problem leads to need for exponential growth in computation time

Can be circumvented by Complex Langevin and Lefschetz Thimbles

Complex Langevin: Clear criteria for whether it works

Complex Langevin works in QCD in all interesting regions

Outlook: Application of Lefschetz thimbles to higher dimensional manifolds $\rightarrow$ make use of symmetries

THE END

Thank you for your attention