

The real-time dynamics of lattice field theories via machine learning

Yukari Yamauchi

arXiv:2101.05755 with Scott Lawrence

10/28/2021, Deep Learning and Physics Online, Japan

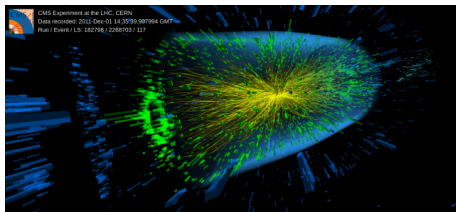
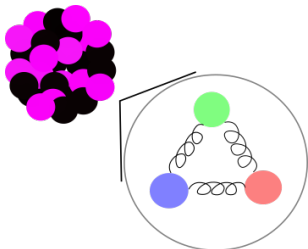


Contents

- ① QCD, Lattice QCD, and Sign problem
- ② Manifold deformation method
- ③ Existence of "perfect manifolds", at least for bosonic theories
- ④ Machine learning based algorithms for finding perfect manifolds

Quantum Chromodynamics

The theory of quarks and gluons:



Tom McCauley/CMS/CERN

$$S_{QCD} = \bar{\psi} (i\gamma^\mu D_\mu - m) \psi - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

Lattice QCD

Non-perturbative method to compute Feynman path integral

Discretize spacetime

$$\text{cutoff } p < \frac{1}{a}$$

Links U take values $g \in SU(3)$

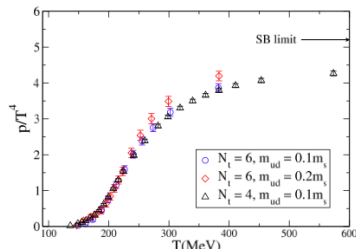
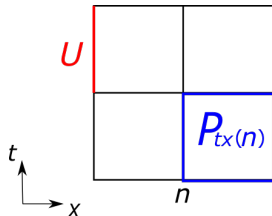
Lattice action (Euclidean, gauge part)

$$S_W = \frac{2}{g_s^2} \sum_{n \in \Lambda} \sum_{\mu < \nu} \text{Re Tr}[1 - P_{\mu\nu}(n)] + O(a^2)$$

Path integral for expectation values

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}[U] e^{-S(U)} \mathcal{O}(U)}{\int \mathcal{D}[U] e^{-S(U)}}$$

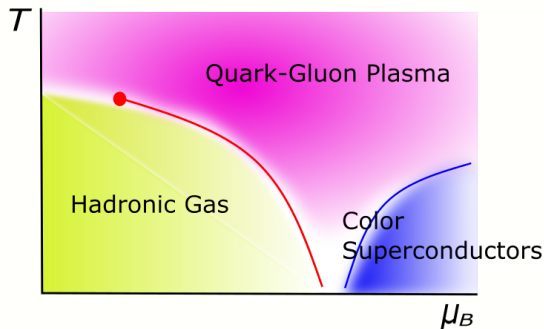
via Markov chain Monte Carlo sampling



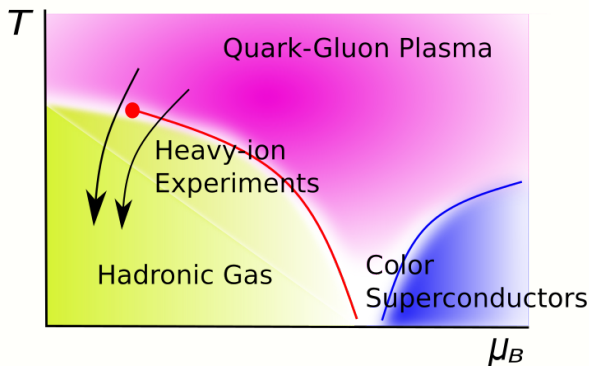
Sign problems

With naive lattice QCD, exponential (in volume) costs to compute

Finite μ_B and **real-time** observables



Shear viscosity of QCD



The shear viscosity η near T_c ¹

$$\frac{1}{4\pi} < \frac{\eta}{s} < \frac{2.5}{4\pi} \text{ for } T_c < T \leq 2T_c$$

¹H. Song, S. A. Bass, U. Heinz, T. Hirano, and C. Shen, Phys. Rev. Lett. 106, 192301 (2011)

Inputs to hydrodynamics

Hydrodynamic fields $\epsilon(\vec{x})$, $u_\mu(\vec{x})$:

$$T_{\mu\nu} = T_{\mu\nu}^{(0)} + T_{\mu\nu}^{(1)} + \dots$$

$$T_{\mu\nu}^{(0)} = (\epsilon + P)u_\mu u_\nu + P g_{\mu\nu}, \quad T_{\mu\nu}^{(1)} = F(\partial_\mu \epsilon, \partial_\mu u_\nu; \eta, \zeta)$$

(P : pressure, η : shear viscosity, ζ : bulk viscosity)

Shear viscosity η :

- From T_{01} correlator:

$$\int_V d\vec{x} e^{i\vec{k}\cdot\vec{x}} \langle \phi(\beta) | [T_{01}(t, \vec{x}), T_{01}(0, 0)] | \phi(\beta) \rangle \sim e^{-\frac{\eta(\beta)k^2}{\epsilon} t}$$

- From T_{12} correlator:

$$\eta(\beta) = \frac{1}{T} \int_V dx \int_0^\infty dt \langle \phi(\beta) | [T_{12}(x, t), T_{12}(0, 0)] | \phi(\beta) \rangle$$

Classical computers \rightarrow Real-time sign problems

Quantum computers \rightarrow No sign problems, but only small computers exist

What can classical computers do?



Euclidean correlators² \rightarrow Error bar on η

Minkowski correlators \rightarrow Real-time sign problem

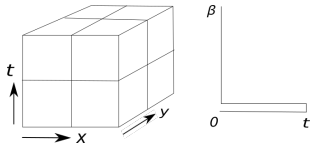
²H. Meyer, Phys.RevD 76 (2007) 101701

Real-time sign problem

Goal: compute $\langle \phi(\beta) | [\mathcal{O}(t, \vec{x}), \mathcal{O}(0, 0)] | \phi(\beta) \rangle$

Method: Lattice QCD via Markov chain Monte Carlo sampling

$$\langle \mathcal{O}(t, \vec{x}) \rangle = \frac{1}{Z} \int \mathcal{D}[\psi, U] e^{-S} \mathcal{O}(t, \vec{x})$$

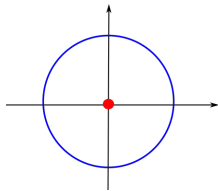


The action S is complex \rightarrow define "quenched distribution" $e^{-\text{Re } S}$

$$\langle \mathcal{O} \rangle = \frac{\langle e^{-i \text{Im } S} \mathcal{O} \rangle_{e^{-\text{Re } S}}}{\langle e^{-i \text{Im } S} \rangle_{e^{-\text{Re } S}}}$$

Especially the **"average sign"** is challenging:

$$\langle \sigma \rangle = \langle e^{-i \text{Im } S} \rangle_{e^{-\text{Re } S}} \propto a^V, \quad |a| \leq 1$$



Toward solving some sign problems⁴

- Manifold deformation method³
- Perfect manifolds ($\langle \sigma \rangle = 1$) in terms of "complex normalizing flows"
- Perfect manifolds (and thus complex normalizing flows) exist!
- How do we find perfect manifolds or complex normalizing flows?
Machine learning?

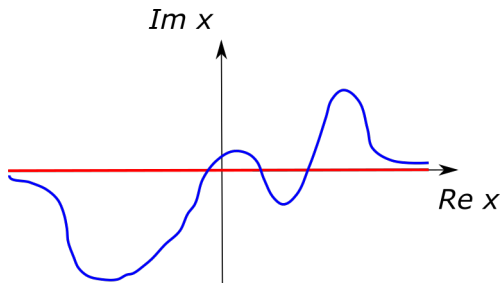
³For review, see A. Alexandru et al., arXiv:2007.05436

⁴S. Lawrence and YY, arXiv:2101.05755

Manifold deformation

One candidate for solving the sign problem is the **Manifold Deformation**

Example: Action $S(x) \rightarrow$ Path integral $\int dx e^{-S(x)}$



$$\langle \sigma \rangle_{\mathcal{M}} = \frac{\int_{\mathcal{M}} e^{-S}}{\int_{\mathcal{M}} e^{-\text{Re } S}} \stackrel{?}{>} \frac{\int_{\mathbb{R}} e^{-S}}{\int_{\mathbb{R}} e^{-\text{Re } S}} = \langle \sigma \rangle_{\mathbb{R}}$$

1D example⁵

The action: $S = x^2 + 2i\alpha x$

$$\langle \sigma \rangle = e^{-\alpha^2}$$

Change the integration contour to

$$z = t - i\alpha, \quad -\infty < t < \infty$$

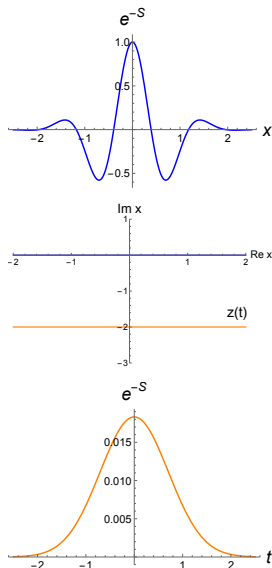
The action on —

$$S(z(t)) = -t^2 - \alpha^2$$

The average sign:

$$\langle \sigma \rangle = \frac{\int dt e^{-\operatorname{Re} S - i \operatorname{Im} S}}{\int dt e^{-\operatorname{Re} S}} = 1$$

No sign problem!!



⁵S. Lawrence, Thesis, arXiv:2006.03683

Perfect manifold and normalizing flow

On a **perfect manifold** $z(t) \subset \mathbb{C}$,

The Boltzmann factor in t :

$$f(t) = \frac{dz}{dt} e^{-S(z(t))}$$

is **real and positive**

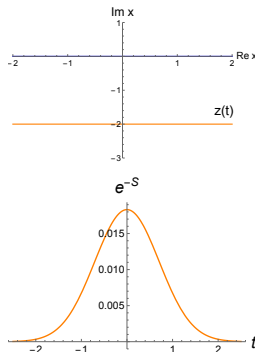
$$\langle \sigma \rangle = \frac{\int dt e^{-S}}{\int dt e^{-\operatorname{Re} S}} = 1$$

$z(t)$ as a map from \mathbb{R} to \mathbb{C} :

$$dz e^{-S(z)} = dt \frac{dz(t)}{dt} e^{-S(z(t))} = dt \mathcal{N} e^{-t^2/2}$$

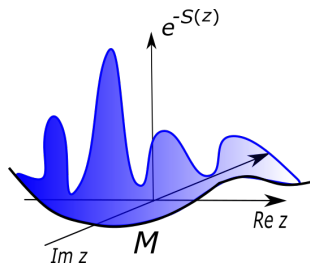
(When S is real, called normalizing flow⁶ \mathbb{R} to \mathbb{R})

Perfect Manifold exists \leftrightarrow Complex normalizing flow $z(t)$ exists



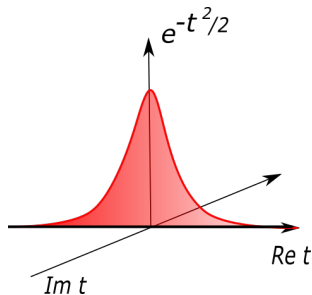
⁶M. Albergo et al. Phys. Rev. D 100, 034515(2019)
K. A. Nicoli, et al. Phys. Rev. E 101, 023304(2020)

Complex normalizing flow



Map

\leftrightarrow
 $z(t)$



Expectation values:

$$\begin{aligned}\langle \mathcal{O} \rangle_{\mathcal{M}} &= \frac{\int_{\mathcal{M}} dz e^{-S(z)} \mathcal{O}(z)}{\int_{\mathcal{M}} dz e^{-S(z)}} = \frac{\int_{\mathbb{R}} dt e^{-t^2/2} \mathcal{O}(z(t))}{\int_{\mathbb{R}} dt e^{-t^2/2}} \\ &\stackrel{?}{=} \frac{\int_{\mathbb{R}} dz e^{-S(z)} \mathcal{O}(z)}{\int_{\mathbb{R}} dz e^{-S(z)}} = \langle \mathcal{O} \rangle\end{aligned}$$

when 3 conditions on \mathcal{M} are met.

Constraints on manifolds⁷

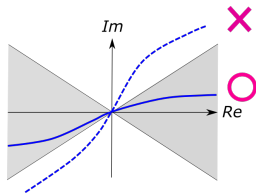
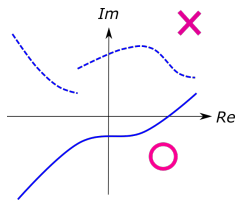
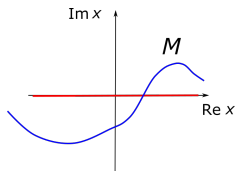
Manifolds give the correct $\langle \mathcal{O} \rangle$

$$\langle \mathcal{O} \rangle = \frac{\int_{\mathbb{R}} dx e^{-S(x)} \mathcal{O}(x)}{\int_{\mathbb{R}} dx e^{-S(x)}} = \frac{\int_{\mathcal{M}} dz e^{-S(z)} \mathcal{O}(z)}{\int_{\mathcal{M}} dz e^{-S(z)}}$$

when:

- The manifold (—) is a continuous manifold
- The manifold (—) is in “asymptotically safe” region
- Both e^{-S} and $e^{-S}\mathcal{O}$ are holomorphic functions in the region between (—) and (—)

→ **Cauchy's integral theorem!**



⁷A. Alexandru et al., Phys. Rev. D. 98, 034506(2018)

Do perfect manifolds exist?

Perfect manifolds exist \leftrightarrow Normalizing flows exist

Do perfect manifolds exist?

If so, can we find them?

If so can use them?

There exist perfect manifolds at least for bosonic theories!

A conjecture on normalizing flows

Type of action: action $S(\vec{z})$ which is finite except at $|\vec{z}| = \infty$

When with **NO** sign problems (S is real)

Fact: Normalizing flows exist. $(\mathbb{R}^N \rightarrow \mathbb{R}^N)$

Conjecture:

Normalizing flows are analytic functions of the parameters of the action.

Example: Scalar field theory $S(\vec{z}; M, \Lambda) = \sum_i z_i M_{ij} z_j + g \Lambda_i z_i^4$ on N sites

The map: $\left(\det \frac{d\vec{z}(\vec{t}; M, \Lambda)}{d\vec{t}} \right) e^{-S(\vec{z}(\vec{t}; M, \Lambda))} = \mathcal{N} \left(e^{-t^2/2} \right)^N$

Perturbative map in weak g :

$$z_i(\vec{t}; M, \Lambda) = z_i - g \left(\sum_j \frac{1}{2} M_{ij}^{-1} \Lambda_j t_j^3 + \frac{3}{4} M_{ij}^{-1} M_{jj}^{-1} \Lambda_j t_j \right)$$

(analytic in M, Λ except at $\det M = 0$)

Perturbative map in strong g is analytic in M, Λ except at $\Lambda = 0$

Existence of perfect manifolds⁸

Conjecture:

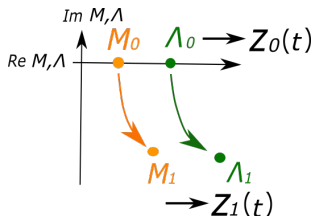
Normalizing flows are analytic functions of the parameters of the action, when $M, \Lambda \in \mathbb{R}$.

Conjecture implies:

Perfect manifolds exist for $M, \Lambda \in \mathbb{C}$

Caveat:

When manifolds intersect with singularity of S , perfect manifolds are not guaranteed to exist



$SU(3)$ Yang-Mills in Minkowski – \bigcirc

Fermionic theories – $?$

Can we find them? If so can we use them?

⁸S. Lawrence and YY, arXiv:2101.05755

Example with scalar field theory⁹

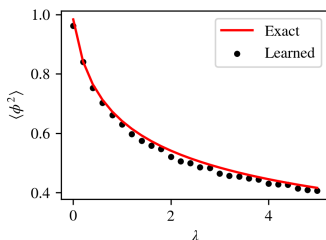
To estimate $\langle \mathcal{O} \rangle_S$ for the action S , let us define $S' = S + \alpha \mathcal{O}$.

A perturbing map $\vec{y}(x)$ from $S'(x + \alpha \vec{y}(x))$ to $S(x)$ satisfies

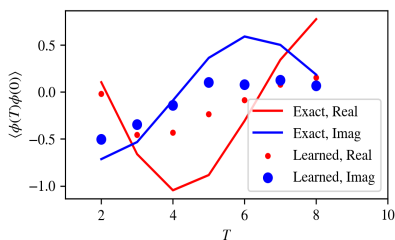
$$\nabla \cdot \vec{y}(x) - \vec{y}(x) \cdot \nabla S(x) - \mathcal{O}(x) + \langle \mathcal{O} \rangle_S = 0$$

Solve the ODE for $\vec{y}(x)$ and $\langle \mathcal{O} \rangle_S$ via machine learning:

$$C(w, \langle \mathcal{O} \rangle_S) = \sum_x |\nabla \cdot \vec{y}_w(x) - \vec{y}_w(x) \cdot \nabla S(x) - \mathcal{O}(x) + \langle \mathcal{O} \rangle_S|^2$$



$0 + 1d, m = 0.5, N_\beta = 10, N_T = 0$



$0 + 1d, m = 0.5, \lambda = 0.5, N_\beta = 2$

⁹S. Lawrence and YY, arXiv:2101.05755

Ongoing work

Establish numerical methods to find flows/manifolds

Normalizing flows:

$$\left(\det \frac{d\vec{z}(\vec{t}; \mathbf{M}, \mathbf{\Lambda})}{d\vec{t}} \right) e^{-S(z(\vec{t}; \mathbf{M}, \mathbf{\Lambda}))} = \mathcal{N} e^{-\vec{t} \cdot \vec{t} / 2}$$

- 1 Represent a normalizing flow with a neural network (parameters \vec{w}).
- 2 Sample \vec{t} from Gaussian distribution.
- 3 The loss function is:

$$L(\vec{w}) = \sum_{\vec{t}} \left| \left(\det \frac{d\vec{z}(\vec{t}; \mathbf{M}, \mathbf{\Lambda})}{d\vec{t}} \right) e^{-S(z(\vec{t}; \mathbf{M}, \mathbf{\Lambda}))} - \mathcal{N} e^{-\vec{t} \cdot \vec{t} / 2} \right|^2$$

- 4 Train the neural network with the loss function.

Thank you!