Machine learning for Lattice gauge theories

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Lattice simulations

High-dimensional path integral over degrees of freedom assigned to points and edges of a lattice

- Boltzmann weight $e^{-S(\phi)}$ encodes distribution over "typical" configurations

Partition function

$$Z \equiv \left[\prod_{x} \int_{-\infty}^{\infty} d\phi(x)\right] e^{-S}$$

Thermal expt. value of operator \mathcal{O}

$$\langle \mathcal{O} \rangle = \left[\prod_{x} \int_{-\infty}^{\infty} d\phi(x) \right] \mathcal{O}(\phi)$$



 $F(\phi)$

 $(\phi) e^{-S(\phi)}/Z$



Why machine learning?

State-of-the-art LGT calculations require enormous computational cost.

- $\gtrsim 10^9$ degrees of freedom
- "Critical slowing down" as $a \rightarrow 0$
- Costly matrix inversion for propagators $\langle \psi \bar{\psi} \rangle$ (especially as $m_q \rightarrow 0$)

This limits the precision of physics results (challenging uncertainties from $a \rightarrow 0$, $m_{\pi} \rightarrow \sim 140 \text{MeV}$, and $V \rightarrow \infty$ limits!)



Why machine learning?

Lattice field theories may be well-suited for application of ML

- Problem involving **lots** of well-structured data
- Analytically-known target
- Generative models with exactness now exist



Stokes, Kamleh, Leinweber 1312.0991

Some applications of ML

Two major components to a lattice calculation. Ongoing efforts to apply ML to both of these.

1. Ensemble generation



Normalizing flow models

- PRD100 (2019) 034515, 2101.08176, 2107.00734
- PRL125 (2020) 121601, ICML (2020) 2002.02428, PRD103 (2021) 074504, 2305.02402
- PRD104 (2021) 114507, PRD106 (2022) 014514, PRD106 (2022) 074506, **PoSLATTICE (2022) 036**
- 2211.07541, 2401.10874, 2404.10819, 2404.11674

See e.g. Boyda, et al. Snowmass 2022, 2202.05838

2. Observable measurements & analysis



Learned contour deformations

- PRD98 (2018) 074511, PoS LATTICE2018 176
- PRD102 (2020) 014514
- PRD103 (2021) 094517
- 2309.00600, NeurIPS ML4PS (2023)



Normalizing flow models

Tabak & Vanden-Eijnden CMS8 (2010) 217 Tabak & Turner CPA66 (2013) 145

- Sample from "easy" prior density $r(\xi)$
- Apply parametrized diffeomorphism f (the "flow")
- Output samples follow new "model density" $q(\phi) = r(\xi) \det |\partial f(\xi) / \partial \xi|^{-1}$
- Flow *f* can be **learned** to match target density!



Example of lattice sampling success



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. . . -2 -1 0 • 2 3

Cost of MCMC vastly reduced due to better topological mixing.

Integral deformations for noisy observables

Lattice integrands are often holomorphic, allowing the integration contour to be deformed without bias.

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{\mathcal{M}} e^{-S(\phi)} \mathcal{O}(\phi) = \frac{1}{Z} \int_{\tilde{\mathcal{M}}} e^{-S(\tilde{\phi})} \mathcal{O}(\tilde{\phi})$$



Detmold, GK, Wagman, Warrington PRD102 (2020) 014514

 Defines a modified observable, which may have improved variance:

 $\mathcal{Q}(\phi) \equiv \det J(\phi) e^{-[S(\tilde{\phi}(\phi)) - S(\phi)]} \mathcal{O}(\tilde{\phi}(\phi))$

$$\langle \hat{Q}(\phi) \rangle = \langle \hat{O}(\phi) \rangle$$

Var[$\hat{Q}(\phi)$] \neq Var[$\hat{O}(\phi)$]



Learning the integration contour The choice of $f: \phi \mapsto \tilde{\phi}$ defines $\tilde{\mathcal{M}}$, $Q(\phi)$, and the variance.



Detmold, GK, Wagman, Warrington PRD102 (2020) 014514, Detmold, GK, Lamm, Wagman, Warrington PRD103 (2021) 094517

- Parameterize $f(\phi; \omega)$ then minimize variance.
 - Caveat: Complex analyticity
 - Caveat: SU(N) variables



