Lattice QCD and other Field Theories

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Summary
Applications of ML/AI for QFTs

- Ensemble generation:
  - Methods already developed by the ML community exist
  - Need adaptation to accommodate physics needs
    - Scalability, Compact variables (SU(3) gauge groups)
  - AI method for tackling the sign problem
    - Encouraging results presented
- Inverse problem:
  - Spectral function reconstruction
  - PDF/GPDs from lattice QCD
- Phase transition identification
- Improved estimators for correlation functions
Presenters

• Akio Tomiya (RIKEN/BNL)
  • Application of ML to computational physics
• Giovanni Pederiva (MSU)
  • Speeding up Hadron Correlator computations with ML
• Kimmy Cushman (Yale)
  • Replacing MCMC with Generative flows
• Andrei Alexandru (GWU)
  • ML for QFTs with a sign problem
• Phiala Shanahan (MIT)
  • ML for LQCD: ensemble generation
Exact algorithm is needed
Self-learning Monte Carlo (SLMC)

SLMC for spin systems

\[ P(S_{k'} | S_k) = \min \left( 1, \frac{e^{-\beta(H[S_k'] - H_{\text{eff}}[S_k'])}}{e^{-\beta(H[S_k] - H_{\text{eff}}[S_k])}} \right) \]

\[ Q^\theta(S_{k'} | S_k) \]

Corrected by modified Metropolis test

Accept/Reject

Proposing part

\[ \theta : \text{tunable parameter} = \text{coupling} \]

Update using effective model

this must satisfy detailed balance

This is an exact algorithm.

Testcase

\[ H = -J \sum_{\langle ij \rangle} S_i S_j - K \sum_{ijkl \in \square} S_i S_j S_k S_l, \]

\[ H_{\text{eff}} = E_0 - \tilde{J}_1 \sum_{\langle ij \rangle_1} S_i S_j \]

\[ S_i = \pm 1 \]

Autocorrelation function

Dynamic Critical exponent

24 time efficient

Very mild scaling
Mock data (vector ch.) from PRD65, 014501(CP-PACS), noise level from Asakawa et al.

\[
\rho_{\text{in}}(\omega) = \frac{2}{\pi} \left[ F_\rho^2 \frac{\Gamma_\rho(\omega)m_\rho}{(\omega^2 - m_\rho^2)^2 + \Gamma_\rho^2 m_\rho^2} + \frac{1}{8} \left( 1 + \frac{\alpha_s}{\pi} \right) \frac{1}{1 + e^{(\omega_0 - \omega)/\delta}} \right].
\]

\[
\Gamma_\rho(\omega) = \frac{1}{48\pi} \frac{m_\rho^3}{F_\rho^2} \left( 1 - \frac{4m_\pi^2}{\omega^2} \right)^{3/2} \theta(\omega - 2m_\pi).
\]

\[
e_{\text{max}} = \frac{1}{2} \left( \frac{\omega_0^2}{\delta^2} + \left( \frac{\omega_0}{\delta} \right)^2 \right).
\]

\[
\rho_{\text{rec}}(\omega) - \rho_{\text{mock}}(\omega) \mid_2 = 0.1071
\]
The main idea of this work is to try to accelerate the computation of the linear system for the quark propagator. We use numerical data for different stopping parameters $\epsilon$ to as training and prediction data sets.

For example, using a precise measurement of the propagator ($\epsilon = 10^{-8}$) on a subset of the ensemble and a less precise (sloppy) one ($\epsilon = 10^{-1}, 10^{-2}, 10^{-3}$) on the whole ensemble.

To properly estimate the uncertainty bias-correction and bootstrap are used.
As a second step, one could try to use more information at the same time. In particular we construct a function to approximate the precise data:

\[ C^F(t) \approx \Gamma^{ML} (C^{e_1}(t), C^{e_2}(t), \ldots, C^{e_n}(t)) \]

where \( C^{e_i}(t) \) is the correlator at precision \( e = 10^{-i} \).
Contour deformation

\[ Z = \int_{-\infty}^{\infty} dx \, e^{-S(x)} \]

\[ S(x) = x^4 - x^2 + 10ix \]

\[ Z = \int_{C} dz \, e^{-S(z)} \]

- Generalized Cauchy’s theorem
- Deformation in the field variable space (lattice geometry unchanged)
Learnifold

- Generate few configs on the generalized thimble manifold
- Use neural nets with appropriate symmetries to interpolate
- Integrate over the learnifold, the manifold defined by the trained neural net
Results

\[ \mathcal{M} = A_0(x) + iA \]

\[ \mathcal{L}_T \]

\[ \langle e^{-iS + \text{Im log det } J} \rangle \]

\[ \langle n \rangle / m_f \]

\[ \mathbb{R}^N \]

\[ \mathcal{M} = A_0(x) + iA \]

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\[ \langle e^{-iS + \text{Im log det } J} \rangle \]

\[ \langle n \rangle / m_f \]

\[ \mathbb{R}^N \]

\[ \mathcal{M} = A_0(x) + iA \]

\[ \mathcal{L}_T \]

FIG. 4. $e^{-iS + \text{Im log det } J}$ and $\langle n \rangle / m_f$ as a function of $\mu/m_f$ for Wilson fermions on lattices of size (top) $10 \times 10$, (center) $20 \times 10$, (bottom) $40 \times 10$ with $am_f = 0.30(1)$. The dashed curve represents the free fermion gas with the same mass. The darker points in the $20 \times 10$ graphs (middle row) correspond to a learnifold trained on $\mathcal{M}$ with $T_{\text{flow}} = 0.4$ whereas the lighter use $T_{\text{flow}} = 0.2$. 

\[ [9] \]


\[ [10] \]


\[ [11] \]


\[ [12] \]


Andrei Alexandru: Sign Problem
Generative models for QCD gauge field generation

Shanahan: Ensemble generation

Machine learning QCD

Massachusetts Institute of Technology

Google

DeepMind

NYU

Center for Theoretical Physics, MIT
Application: scalar field theory

First application: scalar lattice field theory

**Success:** Critical slowing down is eliminated

**Cost:** Up-front training of the model

![Graphs showing the critical slowing down](image)

**Dynamical critical exponents consistent with zero**
Quantitative correlations

\[ C(1, \beta = 1) = 0.53731 \]
\[ \langle \mathcal{O} \rangle = \sum_i \mathcal{O}_i \frac{p_i}{q_i} \bigg|_q \]

unweighted mean = 0.310, \( dx = 1 \)

weighted mean = 0.53421 ± 0.00352
Quantitative correlations

\[ \beta = 0.4 \]
Discussions

• Well-defined avenues for progress have been identified
  • Ensemble generation (with and without a sign problem)
  • Inverse problem

• Increase AI literacy in the LQCD community
  • Organize workshops that focus on the science, summer schools to educate students

• Establish connection between Physics and AI/ML communities

• Funding for small scale initiatives at Labs and Universities

• Support for graduate students, postdocs, bridge faculty positions, lab scientists dedicated to AI/ML applications to LQCD

• Establish relations with ongoing efforts to bring AI to Exascale computing systems (ex. CANDLE project)