Accelerated Monte Carlo methods from machine learning

Yukari Yamauchi

- arXiv:2310.xxxxx with Landon Buskirk, Pablo Giuliani, Kyle Godbey
- arXiv:2310.xxxxx with Scott Lawrence

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Workshop: Probing the Frontiers of Nuclear Physics with AI at the EIC

INSTITUTE for NUCLEAR THEORY

“Accelerating” Monte Carlo sampling for EIC physics

1. Uncertainty quantification via Bayesian analysis

$$P(\omega|\boldsymbol{Y}) = \frac{P(\boldsymbol{Y}|\omega)P(\omega)}{P(\boldsymbol{Y})}$$

   Assisting continuous calibration of model parameters $\boldsymbol{\omega}$ via **normalizing flows**

2. Lattice calculations

$$\langle\mathcal{O}\rangle = \frac{\int \phi \exp(-S_0(\phi))\ \mathcal{O}(\phi)}{\int_\phi \exp(-S_0(\phi))}$$

   Increasing effective sampling size via **control variates**

Bayesian analysis with normalizing flows

Bayes theorem provides posterior distribution

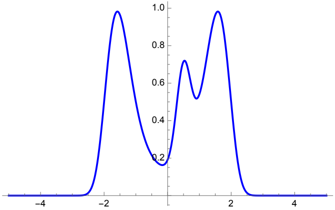
$$P(\omega|\boldsymbol{Y}) = \frac{P(\boldsymbol{Y}|\omega)P(\omega)}{P(\boldsymbol{Y})}$$

How do we sample from $P(\omega|\boldsymbol{Y})$? Normally MCMC

Normalizing flow $\omega = f(\boldsymbol{x})$ maps

$$d\omega\ P(\omega|\boldsymbol{Y}) = \mathcal{N} \prod_{i=1}^{N} dx_i\ e^{-x_i^2/2}$$

Some distribution

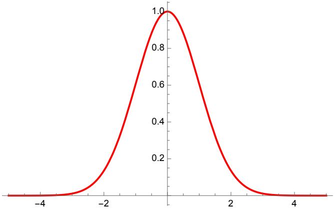


Map

$$\leftrightarrow$$

$$\omega = f(\boldsymbol{x})$$

Gaussian distribution



Mahcine-learned normalising flow

Find an approximate normalizing flow

$$\mathcal{N} \prod_{i=1}^{N} dx_i \; e^{-x_i^2/2} = d\omega \; Q(\omega) \approx d\omega \; P(\omega|\boldsymbol{Y})$$

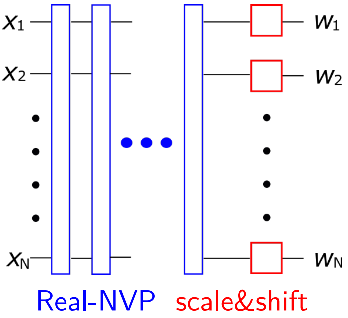
by optimizing parameters in the neural network

Real NVP (6 layers) + Scale&Shift

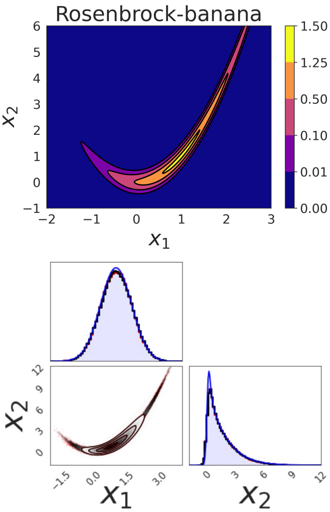
1. Prepare train data via MCMC
2. Initialize NN as a Gaussian fit
3. Train via Jeffreys' divergence

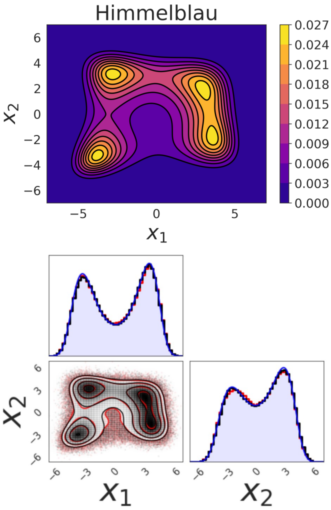
$$D(P|Q) = \int d\omega \left(\tilde{P} \log \frac{P}{Q} + \tilde{Q} \log \frac{Q}{P} \right)$$

- Adam with learning rate of 10^{-3}
- 1000 samples/train step



2-dimentional examples

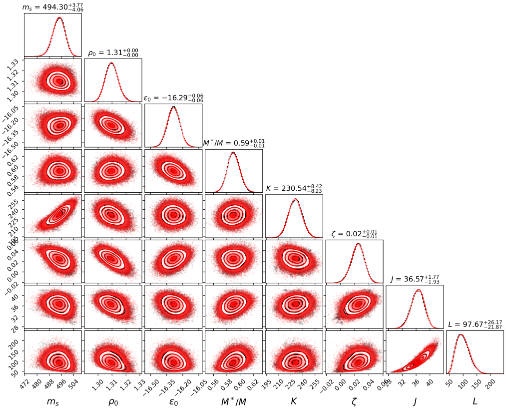




blue: exact, **black**: train data, **red**: from normalizing flow

Relativistic mean field model[3]

Calibrated by experimental binding energies and charge radii of nuclei[1]
(^{16}O, ^{40}Ca, ^{48}Ca, ^{68}Ni, ^{90}Zr, ^{100}Sn, ^{116}Sn, ^{132}Sn, ^{144}Sm, ^{208}Pb)



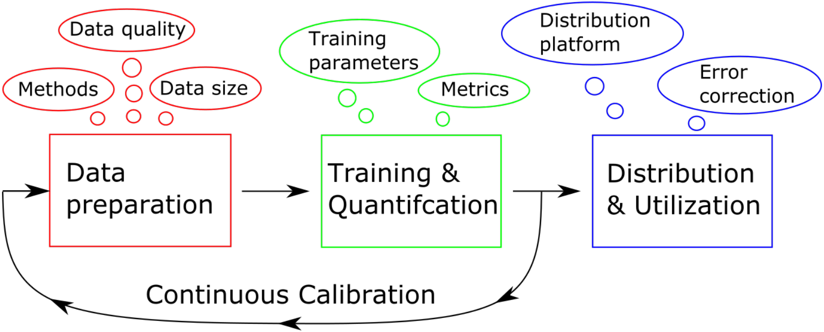
- m_s: σ meson mass
- ρ_0: saturation density
- ϵ_0: binding energy at ρ_0
- M^*: effective nucleon mass at ρ_0
- K: incompressibility at ρ_0
- J: value of symmetric energy at ρ_0
- L: slope of symemtric energy at ρ_0
- ζ: ω meson quartic coupling

Black: MCMC, Red: NF

All codes used in this work will become available at publication[2]

[1] P. Giuliani, K. Godbey, et al., arXiv:2209.13039[nucl-th]
[2] **YY**, L. Buskirk, P. Giuliani, and K. Godbey, in preparation
[3] W. Chen and J. Piekarewicz, arXiv:1408.4149

Why normalizing flow? Why with machine learning?



- Neural network can parametrize a large family of functions efficiently.
- Normalizing flows serve as a compression tool for $P(\boldsymbol{\omega}|\boldsymbol{Y})$.
- One can generate more samples easily, quickly, in parallel (including reweighting).

Next!

Improving the statistics in lattice calculations via **control variates**

For a given Monte Carlo sampling task in lattice simulations

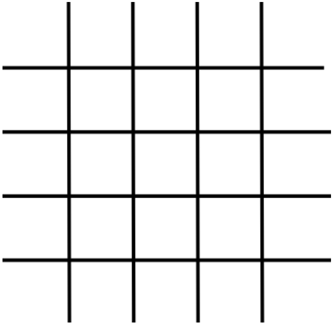
$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}[\phi]\ e^{-S(\phi)}\ \mathcal{O}(\phi)}{\int \mathcal{D}[\phi]\ e^{-S(\phi)}}$$

with bad

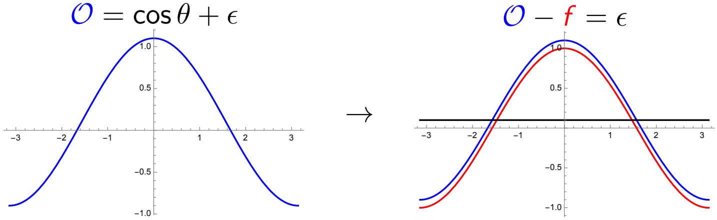
Signal-to-noise problem

How do we reduce the "noise"

Variance $\mathrm{Var}(\mathcal{O})$



Complex control variates



The idea is very simple...

Subtract a function f from $\mathcal{O}$!!

Without changing physics, so

$$\langle \mathcal{O} \rangle = \langle \mathcal{O} - f \rangle \;\text{ but }\; \mathrm{Var}(\mathcal{O}) > \mathrm{Var}(\mathcal{O} - f)$$

So we strictly impose

$$\langle f \rangle = \int \mathcal{D}[\phi]\, e^{-S(\phi)}\, f(\phi) = 0$$

Notes on control variates

Strength of control variates

- Can be applied to any (including discrete) lattice theories
- Good (or even perfect) control variates always exist

How do we find good control variates?

1. Analytical (perturbative) approaches
   - S. Lawrence, arXiv:2009.10901[hep-lat]
   - S. Lawrence and **YY**, arXiv:2212.14606 [hep-lat]

2. Numerical approaches
   - Start with ansatz and optimize
   - Machine learning

Demonstration: Classical Ising model (Lee-Yang zeros)

Classical Ising model: $S(\vec{s}) = -J\sum_{\langle i,j\rangle} s_i s_j - h\sum_i s_i$

Lee-Yang Theorem: the partition function is **0** only on with imaginary h.

Goal: Compute $Z = \sum_s e^{-S}$ at **purely imaginary magnetic field**

Measure

$$\frac{Z(h)}{Z(h=0)} = \frac{\sum_s \exp\Big(J\sum_{\langle i,j\rangle} s_i s_j\Big)\ \exp\big(h\sum_i s_i\big)}{\sum_s \exp\Big(J\sum_{\langle i,j\rangle} s_i s_j\Big)} = \left\langle e^{h\sum_i s_i}\right\rangle_Q$$

By replacing

$$e^{h\sum_i s_i} \to e^{h\sum_i s_i} - \textbf{CV}$$

and optimize **CV** to minimize

$$\mathrm{Var}\left(e^{h\sum_i s_i} - \textbf{CV}\right)$$

Extreme learning machine

1. Prepare basis functions

$$\left\{\sum s, \cos(\sum s), \sin(\sum s)\right\} \times s \times S(h=0)^n$$

$(0 \leq n \leq 3)$

2. Input basis functions to ELM

3. Take "divergence"

$$F_i = f(s_i) - f(-s_i)$$

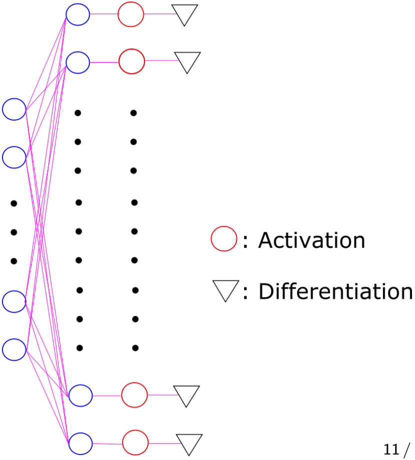
4. The $CV = \sum_i c_i F_i$

The coefficients c_i are optimized by estimating

$$M_{ij} = \langle F_i F_j \rangle, v_j = \langle \mathcal{O} F_i \rangle$$

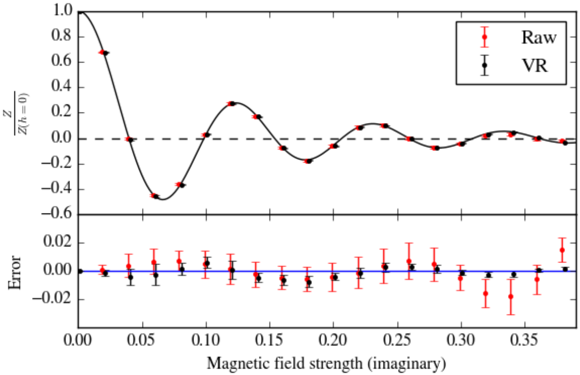
and

$$c = M^{-1}\ v$$



Classical Ising model[4]

At purely imaginary h, $J = 0.4 < J_c \approx 0.441$, 8×8 lattice:



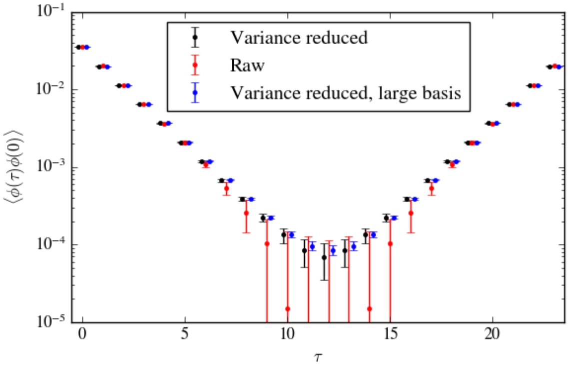
- Raw: 5k samples for Z
- VR: 5k samples to optimize, 5k samples for Z

[4]S. Lawrence and **YY**, in preparation

Scaler field theory[5]

Lattice scalar ϕ^4 theory in Euclidean

$$S = \sum_{\langle r,r'\rangle} \frac{(\phi(r)-\phi(r'))^2}{2} + \sum_r \left[\frac{m^2}{2}\phi^2(r) + \frac{\lambda}{24}\phi^4(r)\right]$$



24×24 lattice, $m^2 = 0.0, \lambda = 2.0$

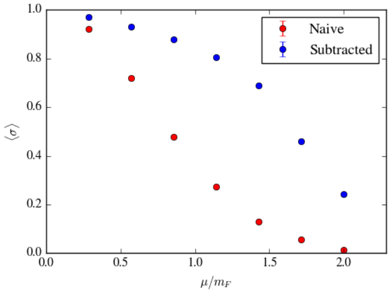
[5] T. Bhattacharya, S. Lawrence, and J. Yoo, arXiv:2307.14950 [hep-lat]

Thirring model in $1+1$-dimension at finite density [6]

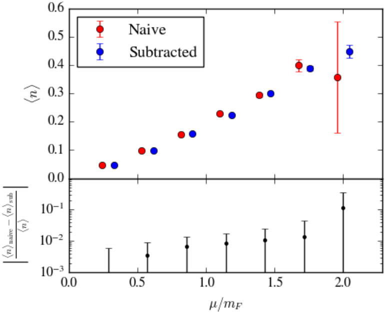
$$S = \sum_{x,\nu} \frac{2}{g^2} \left(1 - \cos A_\nu(x)\right) - \log\det K,\, A_\nu \in [0, 2\pi)$$

with the Dirac matrix ($\eta_0 = (-1)^{\delta_{0,x_0}}$ and $\eta_1 = (-1)^{x_0}$)

$$K[A]_{xy} = m\delta_{xy} + \frac{1}{2}\sum_{\nu=0,1} \eta_\nu e^{iA_\nu(x)+\mu\delta_{\nu,0}}\delta_{x+\nu,y} - \eta_\nu e^{-iA_\nu(y)-\mu\delta_{\nu,0}}\delta_{y+\nu,x}$$



Average sign



Density

4×4 lattice, $m = 0.05, g = 1.0 \to m_B = 0.33(1), m_F = 0.35(2)$

[6] S. Lawrence and **YY**, arXiv:2212.14606 [hep-lat]

Future

Bayesian analysis via NF

- Efficient training algorithms
- Continuous calibration

Lattice control variates

- Application to LQCD
- Towards sign problems

Collaborators (?)

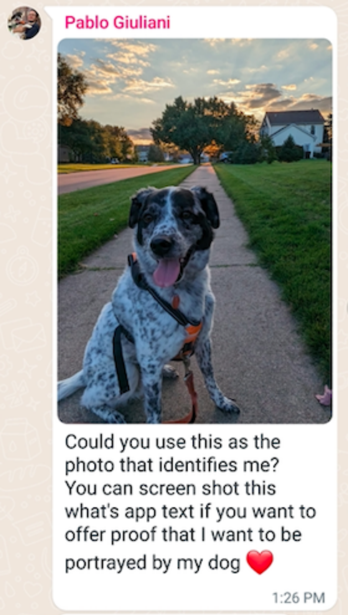
Landon Buskirk

Pablo Giuliani

Kyle Godbey

Scott Lawrence

BACK UP


Pablo Giuliani
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