AI tools for lattice QCD computations

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RBRC Virtual Workshop: Small-x Physics in the EIC Era

December 16, 2021

Outline

Lattice QCD (LQCD)

- Lightning review
- How is progress made in LQCD?
- LQCD for small-x physics?

Machine learning (ML)

- How can we employ ML?

Application: normalizing flows for LQFT sampling

- Framework
- Progress towards LQCD
- Access to new sorts of observables(?)

Outlook

Lattice QCD (LQCD)

Only known controlled, systematically improvable way to investigate non-perturbative dynamics

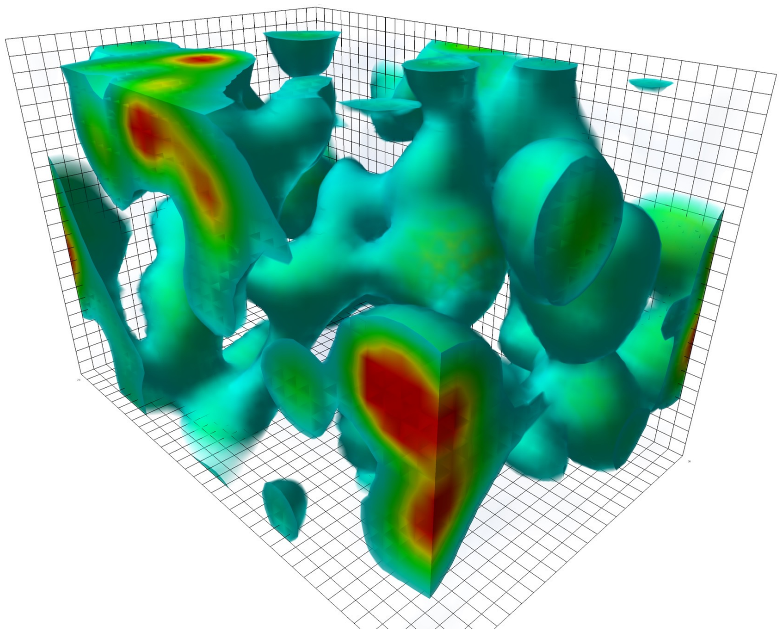
QCD path integral:

$$Z = \int \mathcal{D}[A, \psi, \bar{\psi}] \; e^{i\, S[A,\psi,\bar{\psi}]}$$

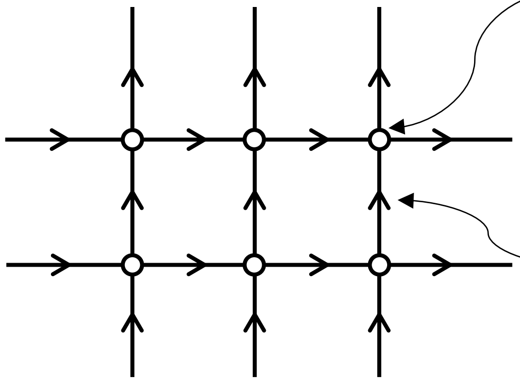
1. Wick rotate: $iS \to -S_E$
   (3+1)d Minkowski → 4d Euclidean
2. Discretize fields (UV regulator)
3. Restrict to finite box (IR regulator)

$$Z = \int d[U, \psi, \bar{\psi}] \; e^{-S(U,\psi,\bar{\psi})}$$

Result: finite, multidimensional integral
→ Evaluate numerically using MCMC



Visualizations of Quantum Chromodynamics



LQCD Calculation Workflow

1. Configuration generation

   Use MCMC to draw samples (gauge configurations) from $p(U) \propto e^{-S_E(U)}$

   Computationally intensive

   …and gets increasingly expensive for finer lattices

2. Measurement

   Evaluate observables on each config

   e.g. hadronic two-point functions $\sim \langle \bar{\chi}(x)\chi(0)\rangle$

   e.g. hadronic three-point functions $\sim \langle \bar{\chi}(x)\, J(y)\, \chi(0)\rangle$

   Also expensive

3. Analysis

   Must relate Euclidean-time matrix elements to real-world QCD

MCMC expectations

$$\langle O \rangle \approx \frac{1}{N}\sum_{i=1}^{N} O(U_i)$$

Asymptotically unbiased

⇒ Exactness guaranteed

Advancement in LQCD

Algorithmic

Make new calculations tractable

Examples:

Hybrid Monte Carlo (HMC)

→ Controlled treatment of fermions

Conjugate gradient preconditioners

e.g. mass/Hasenbusch

e.g. algebraic multigrid

→ Lighter/physical quark masses

Formal

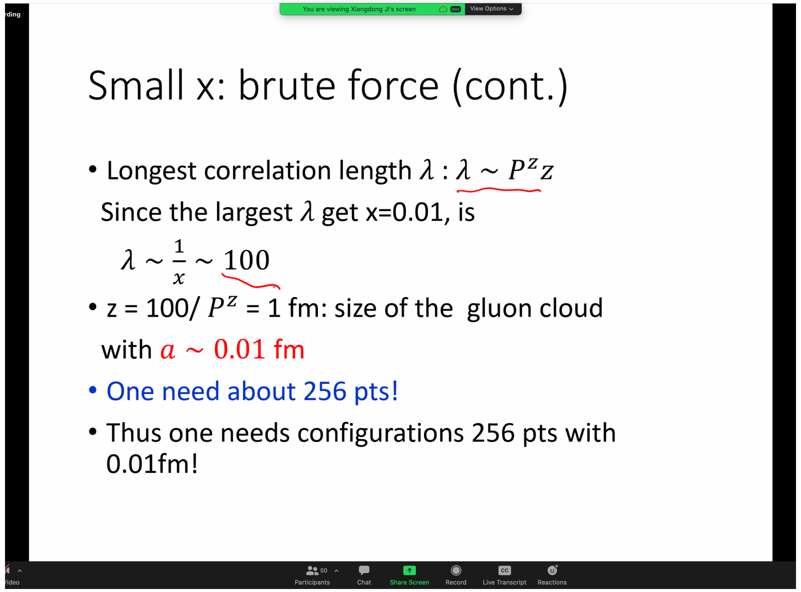
New kinds of calculations

Example:

LaMET / quasi PDFs

SDF / pseudo PDFs

(Challenges for) LQCD for small x



LaMET / quasi PDFs: see Ji's talk yesterday

"Small x: brute force" resource requirements [Ji's talk]:

$a \sim 0.01$ fm and $L/a \sim 256$ for $x \sim 0.01$

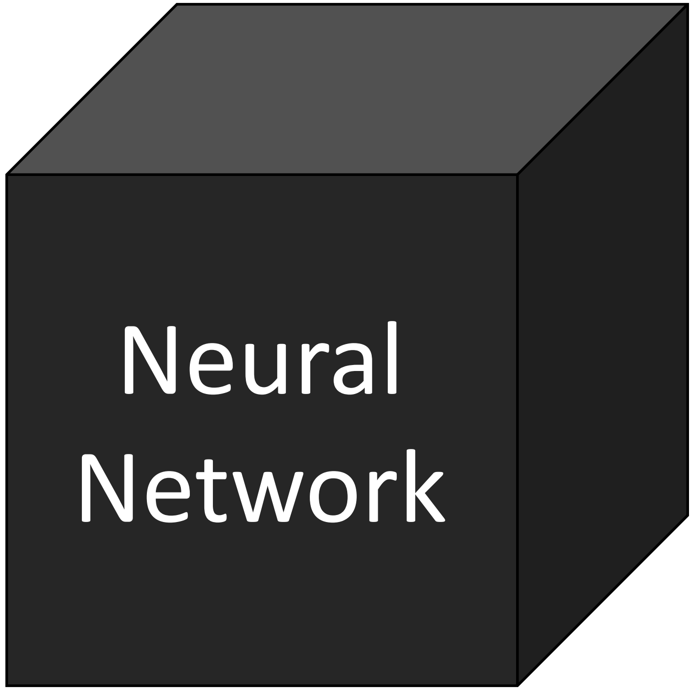
→ Difficult for modern LQCD

Other approaches:

Reconstructing x dependence from Mellin moments

(many more)

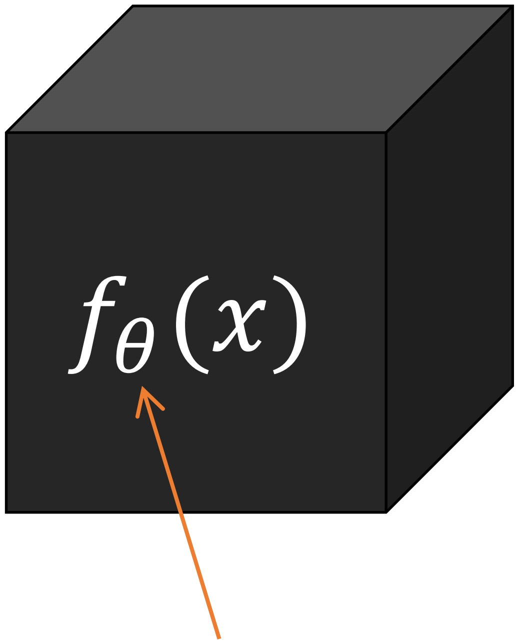
Machine learning



ML for LQCD?

Open research questions:

1. Where can we use black boxes without compromising exactness?
2. How can we build physics knowledge into NNs / ML models?



θ = optimizable parameters

ML for LQCD: recent work (non-exhaustive)

Configuration Generation, not including (lots of) other work on ML for measurement, analysis

Flow-based generative models for Markov chain Monte Carlo in lattice field theory
Albergo, Kanwar, Shanahan 1904.12072

Equivariant flow-based sampling for lattice gauge theory
Kanwar, Albergo, Boyda, Cranmer, DH, Racanière Rezende, Shanahan 2003.06413

Sampling using SU(N) gauge equivariant flows
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Flow-based sampling for multimodal distributions in lattice field theory
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Estimation of Thermodynamic Observables in Lattice Field Theories with Deep Generative Models
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Efficient modeling of trivializing maps for lattice ϕ^4 theory using normalizing flows: A first look at scalability
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Reducing Autocorrelation Times in Lattice Simulations with Generative Adversarial Networks
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Towards reduction of autocorrelation in HMC by machine learning
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Gauge covariant neural network for 4 dimensional non-abelian gauge theory
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Adaptive Monte Carlo augmented with normalizing flows
Gabrié,Rotskoff, Vanden-Eijnden
https://arxiv.org/abs/2105.12603

Exploring cluster Monte Carlo updates with Boltzmann machines
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HMC with Normalizing Flows
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LeapfrogLayers: A Trainable Framework for Effective Topological Sampling
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Scaling Up Machine Learning For Quantum Field Theory with Equivariant Continuous Flows
de Haan, Rainone, Cheng, Bondesan 2110.02673

Normalizing Flows and the Real-Time Sign Problem
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Deep Learning Beyond Lefschetz Thimbles
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Machine learning to alleviate Hubbard-model sign problems
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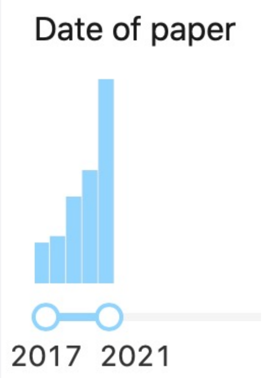

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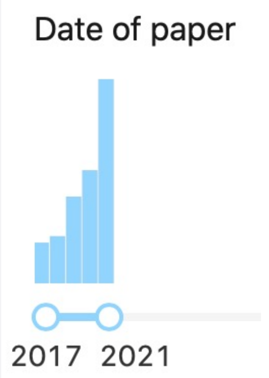
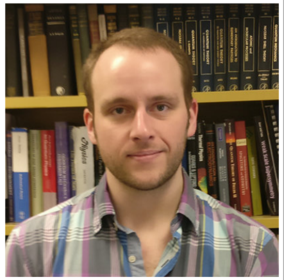


Collaborators (non-exhaustive)

Massachusetts Institute of Technology

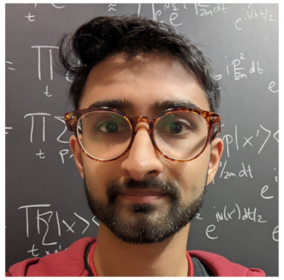

Phiala Shanahan


Dan Hackett


Denis Boyda

Argonne NATIONAL LABORATORY

UNIVERSITÄT BERN


Gurtej Kanwar

UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386


Julian Urban

NEW YORK UNIVERSITY


Kyle Cranmer


Michael Albergo


Chung-Chun Hsieh

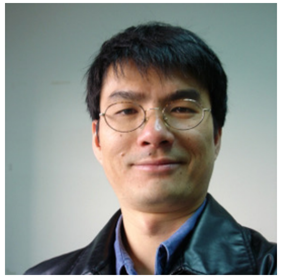
UNIVERSITY OF MARYLAND 1856

DeepMind


Sébastien Racanière


Danilo Rezende


Kai-Feng Chen


Jiunn-Wei Chen

Normalizing Flows

ML method to construct samplers for complicated probability distributions

Sampling from the model distribution:

1. Draw noise z from base distribution w/ density $r(z)$
2. Apply flow f_θ to obtain sample from model $U = f_\theta(z)$

Model density given by conservation of probability:

$$q_\theta(U) = \left|\det \frac{\partial f_\theta(z)}{\partial z}\right|^{-1} r(z)$$

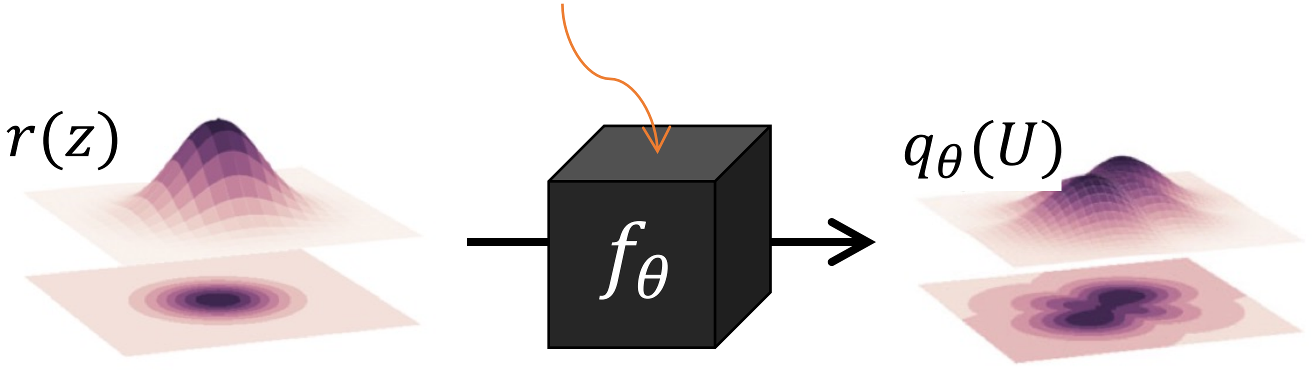
→ sufficient info to compute unbiased expectations

Reweighting: $\langle O \rangle \approx \frac{1}{N}\sum_i \frac{p(U_i)}{q(U_i)} O(U_i)$

Or: use as proposals for MCMC

"Flow"

- Invertible transformation of field dof
- Parametrized by NNs (trainable, expressive ansatz)
- Tractable Jacobian determinant



Simple **base distribution** r

- Easy to sample $z \sim r$
- Easy to compute density $r(z)$

Learned **model distribution** q_θ

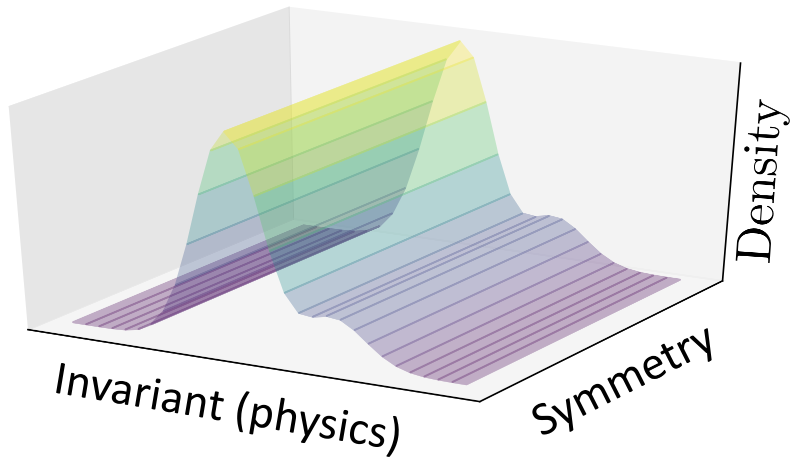
Building symmetries into ML models

Symmetries ⇔ Constraints between model parameters

→ must be learned

→ training more computationally expensive, less stable

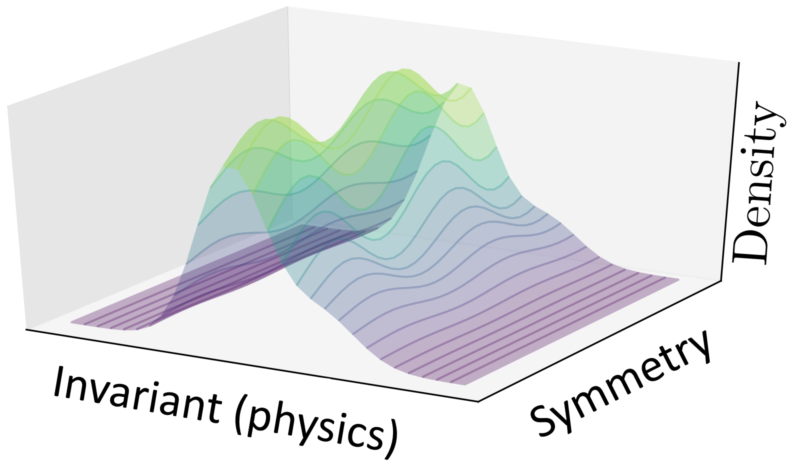
Instead: put constraints in by hand



True distribution

General approach: invariant models/equivariant flows

1. *Invariant* base distribution: $r(\phi) = r(t(\phi))$
2. *Equivariant* flow $f\big(t(\phi)\big) = t(f(\phi))$



Approximation learned by symm-naive ML model

Examples

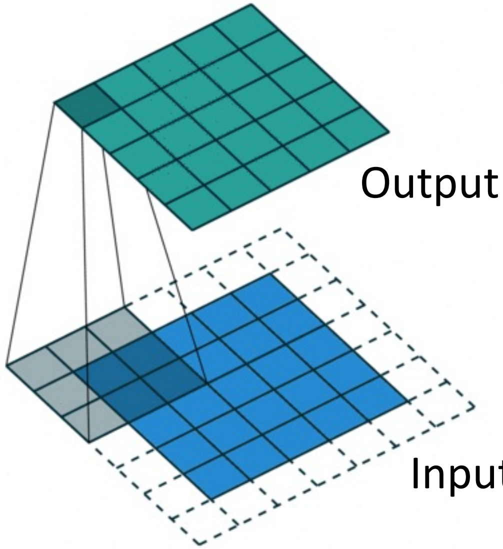
Translational symmetry

1. Invariant base distribution: same for each site
2. Equivariant flow: parametrized by CNNS

   Bosons: PBCs (out-of-the-box circular padding)

   Fermions: antiperiodic in time, PBCs in space

   [Albergo, Kanwar, Racanière, Rezende, Urban, Boyda, Cranmer, DH, Shanahan 2106.05934]



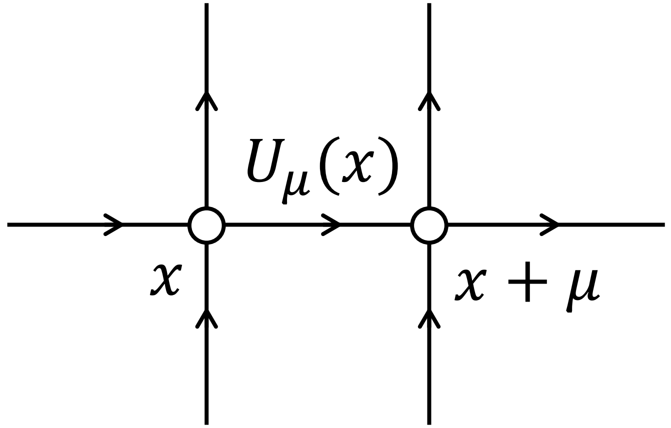
[Image from freecodecamp.org]

Gauge invariance

1. Base distribution: Haar measure
2. Gauge equivariant flow

   U(1): [Kanwar, Albergo, Boyda, Cranmer, DH, Racanière, Rezende, Shanahan 2003.06413]

   SU(N): [Kanwar, Albergo, Boyda, Cranmer, DH, Racanière, Rezende, Shanahan 2003.06413]



$$U_\mu(x) \to \Omega^\dagger(x+\mu)\, U_\mu(x)\, \Omega(x)$$

Climbing the theory ladder

(1+1)d real scalar field theory

[Albergo, Kanwar, Shanahan 1904.12072]

Broken phase: [DH, Hsieh, Albergo, Boyda, JW Chen, KF Chen, Cranmer, Kanwar, Shananan 2107.00734]

(1+1)d Abelian gauge theory

[Kanwar, Albergo, Boyda, Cranmer, DH, Racanière, Rezende, Shanahan 2003.06413]

(1+1)d non-Abelian gauge theory

[Kanwar, Albergo, Boyda, Cranmer, DH, Racanière, Rezende, Shanahan 2003.06413]

(1+1)d Yukawa model

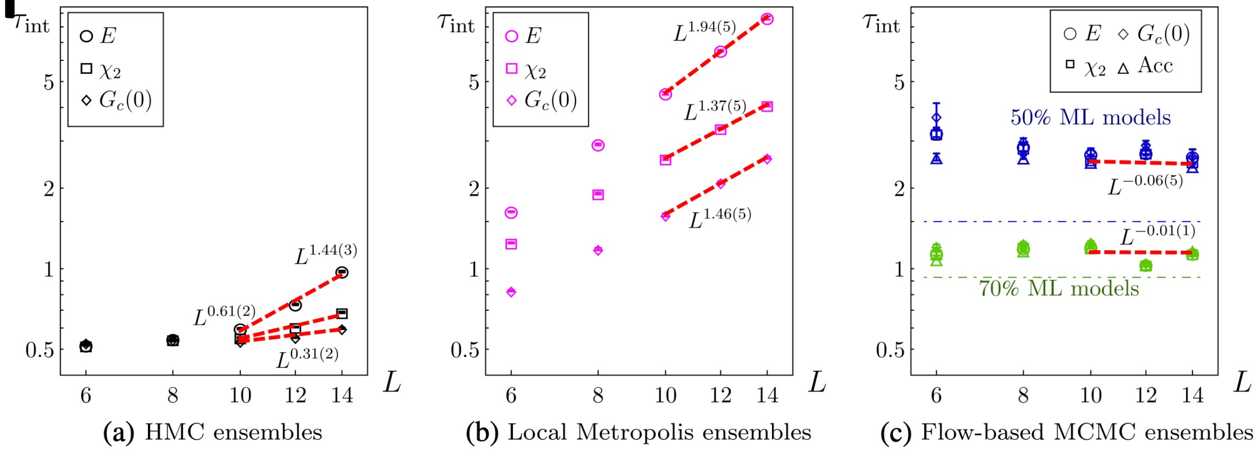
i.e. real scalar field theory + fermions

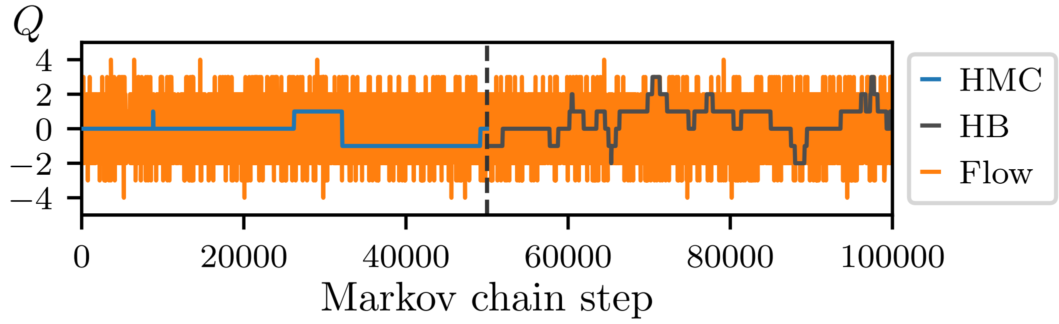
[Albergo, Kanwar, Racanière, Rezende, Urban, Boyda, Cranmer, DH, Shanahan 2106.05934]

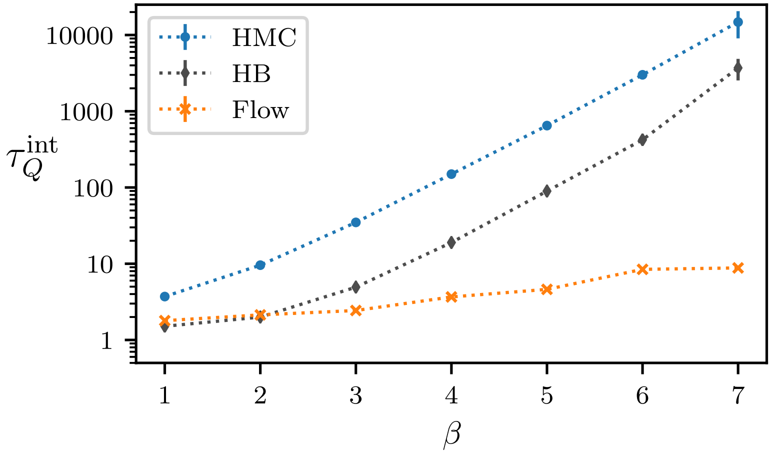
...

QCD!

Real scalar field theory







(1+1)d U(1) gauge theory

Novel capability: direct access to partition function

[Nicoli, Anders, Funcke, Hartung, Jansen, Kessel, Nakajima, Stornati 2007.07115]

Only know how to compute unnormalized $p(U)$

$$p(U) = \frac{e^{-S(U)}}{Z}$$

$S(U)$ ← Known, tractably computable function of the fields

Z ← Intractable (using traditional MCMC algos)

but: flow model density $q(U)$ is normalized

→ unbiased stochastic estimate of Z using flow model samples

$$Z \approx \frac{1}{N} \sum_i \frac{e^{-S(U_i)}}{q(U_i)}$$

Example use case: *direct* estimation of thermodynamic observables (i.e. finite-T equation of state)

Much simpler, more controlled than existing techniques

Outlook

Small x physics are challenging for LQCD

...but better algorithms and new ideas will help

ML for LQCD

Possible to use ML without compromising exactness

ML provides new opportunities for algorithmic & formal advances

Early results with normalizing flows show great promise

Only beginning to explore what's possible; stay tuned.