Lattice QCD and other Field Theories

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Summary

Aplications 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 tranistion 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

J.Liu, Y.Qi, Z.Meng, L.Fu (arXiv:1610.03137)

Accept/Reject **Proposing part**

θ : tunable parameter = coupling

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

Corrected by modified Metropolis test

Update using effective model this must satisfy detailed balance

This is an exact algorithm.

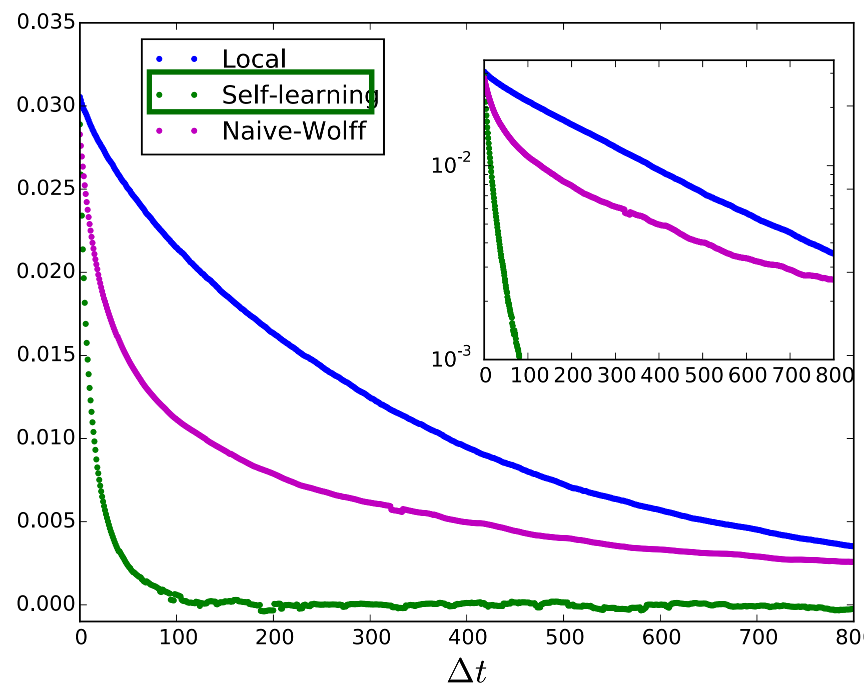
Testcase

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

$$H_{\rm eff} = E_0 - \tilde{J}_1 \sum_{\langle ij\rangle_1} S_i S_j$$

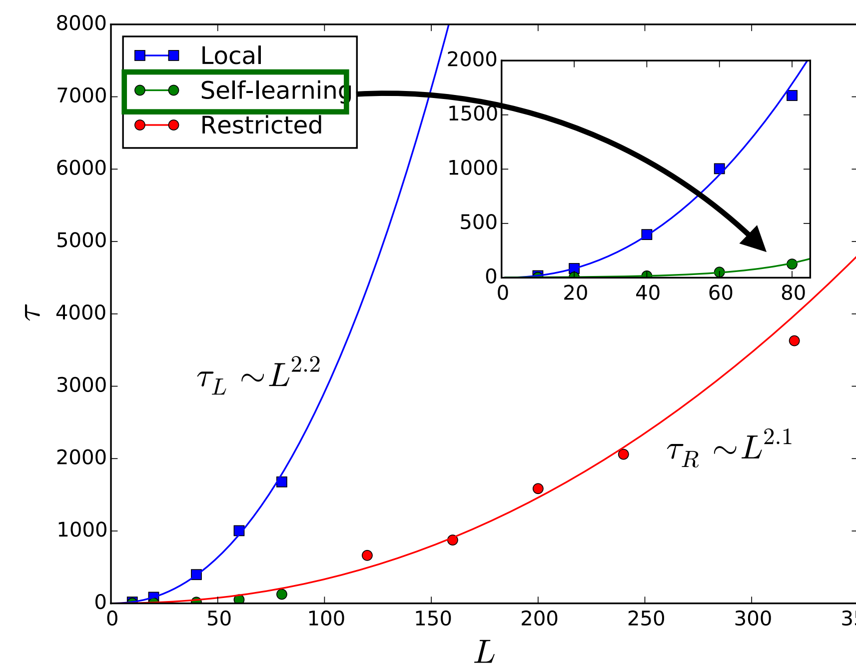
$$S_i = \pm 1$$

Autocorrelation function



24 time efficient

Dynamic Critical exponent



Very mild scaling

(very) Preliminary results

Mock data + noise: it is well reconstructed …?

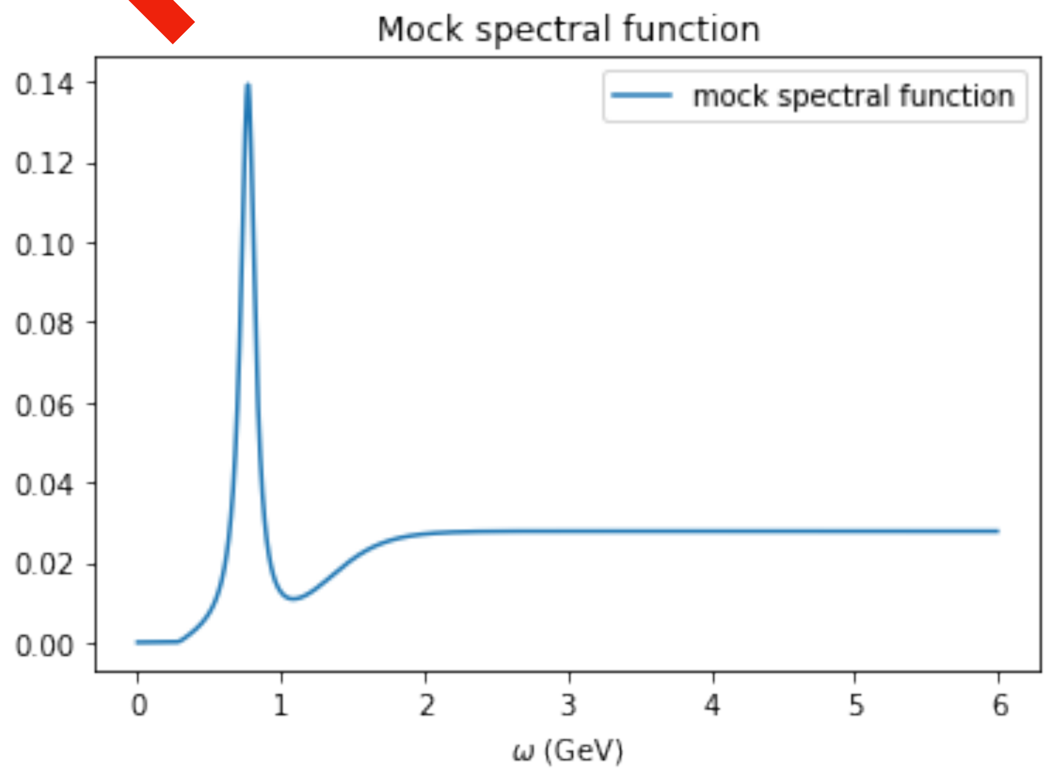
Mock data (vector ch.) from PRD65, 014501(CP-PACS), noise level from Asakawa et al.

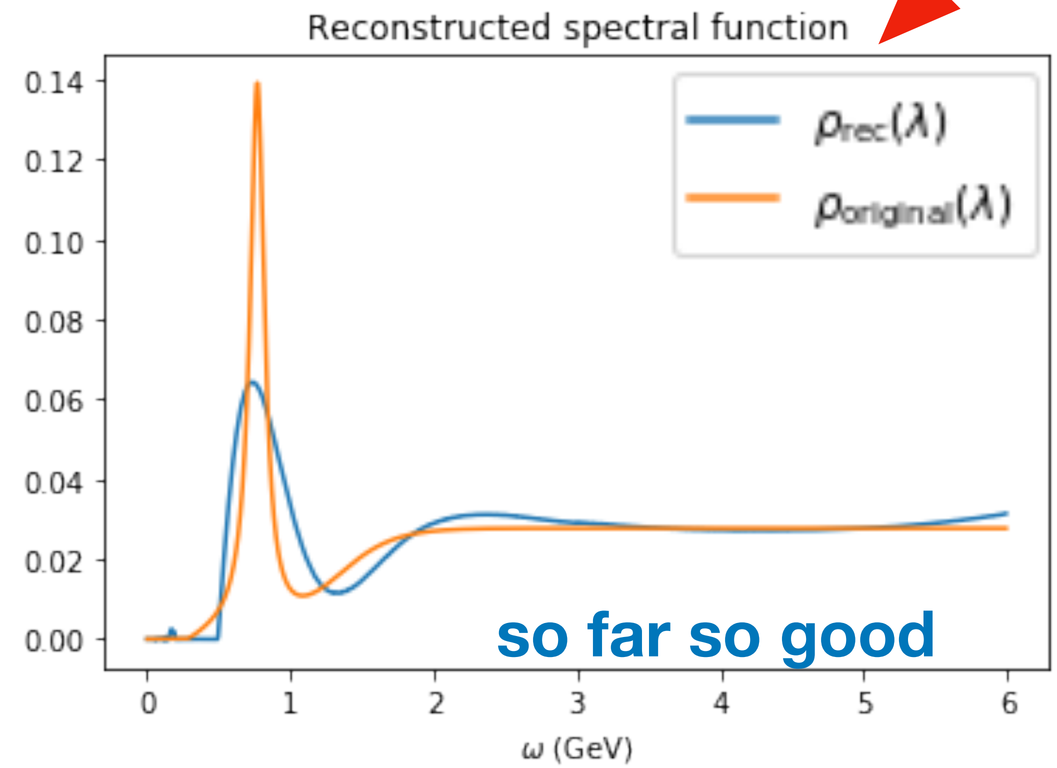
$$\rho_{in}(\omega) = \frac{2}{\pi}\left[F_\rho^2 \frac{\Gamma_\rho(\omega) m_\rho}{(\omega^2 - m_\rho^2)^2 + \Gamma_\rho^2(\omega) m_\rho^2} + \frac{1}{8\pi}\left(1 + \frac{\alpha_s}{\pi}\right)\frac{1}{1 + e^{(\omega_0 - \omega)/\delta}}\right].$$

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

$$m_\rho = 0.77, \quad m_\pi = 0.14, \quad F_\rho = 0.142,$$
$$\omega_0 = 1.3, \quad \delta = 0.2, \quad \alpha_s = 0.3,$$

ρ(mock data) $\xrightarrow[\text{w/ kernel}]{\text{integration}}$ **G** $\xrightarrow[\text{“Mimic MC”}]{\text{+Gaussian noise}}$ **G+noise** $\xrightarrow[\text{in SVD basis}]{\text{Sparse modeling}}$ **ρ(reconstruct)**



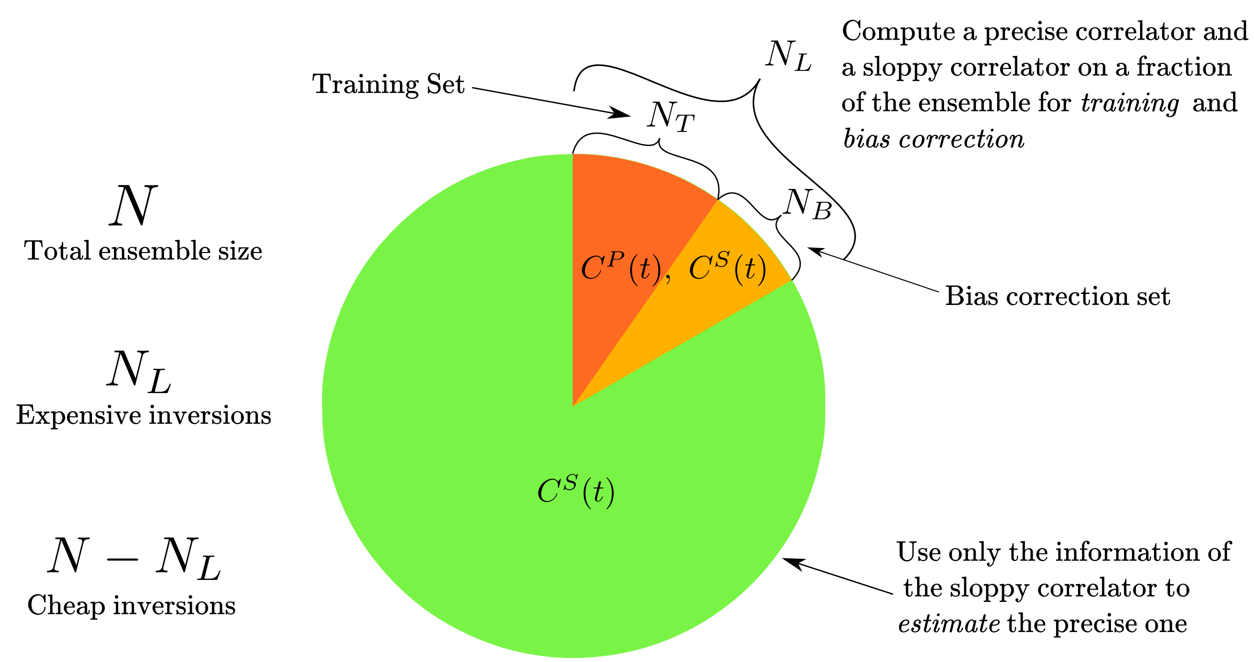


$$|\rho_{rec}(\omega) - \rho_{mock}(\omega)|_2 = 0.1071$$

The Goal

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 ϵ to as training and prediction data sets.

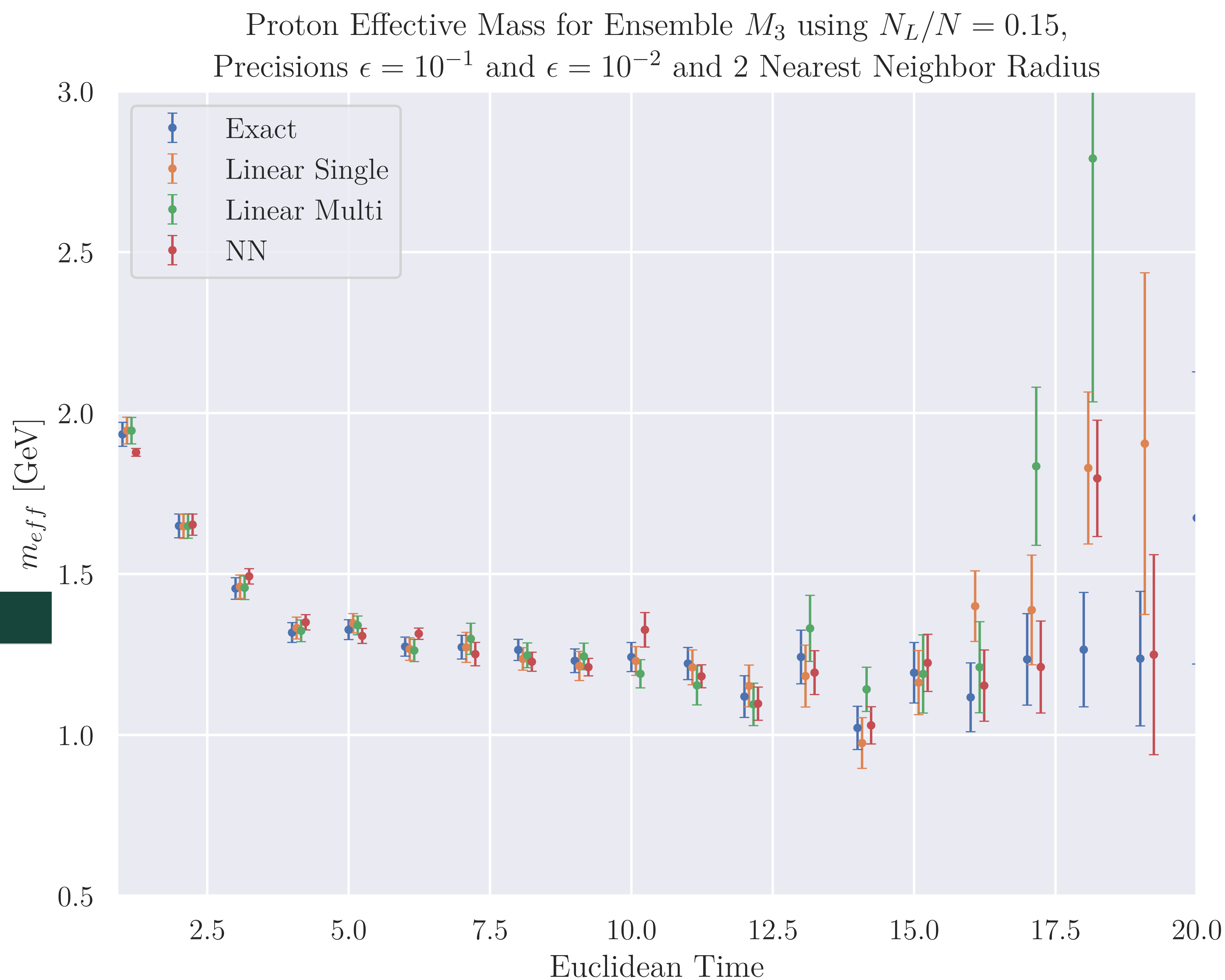
For example, using a precise measurement of the propagator ($\epsilon = 10^{-8}$) on a subset of the ensemble and a less precise (sloppy) one ($\epsilon = 10^{-1}, 10^{-2}, 10^{-3}$) on the whole ensemble.



To properly estimate the uncertainty bias-correction and boostrap are used.

Giovani Pederiva

Using more information at once, nearest neighbors

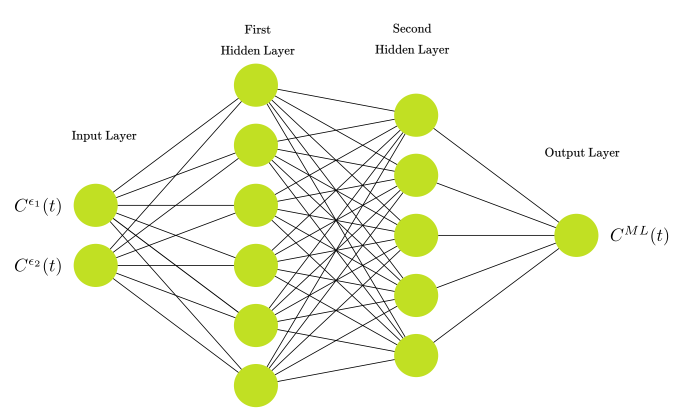


Using more information at once

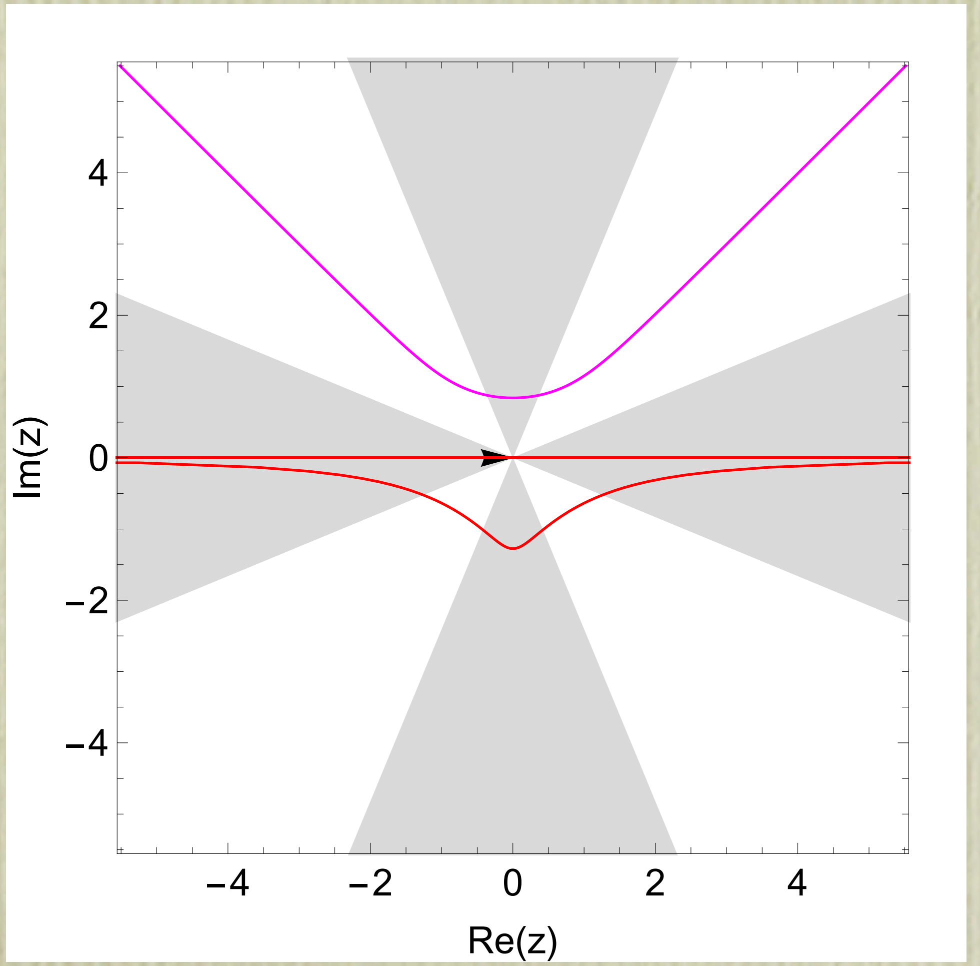
As a second step, one could try to use more information at the same time. In particular we construct a function to approximate the precise data:

$$C^P(t) \approx \Gamma^{ML}\left(C^{\epsilon_1}(t), C^{\epsilon_2}(t), ..., C^{\epsilon_n}(t)\right)$$

where $C^{\epsilon_i}(t)$ is the correlator at precision $\epsilon = 10^{-i}$.



Contour deformation



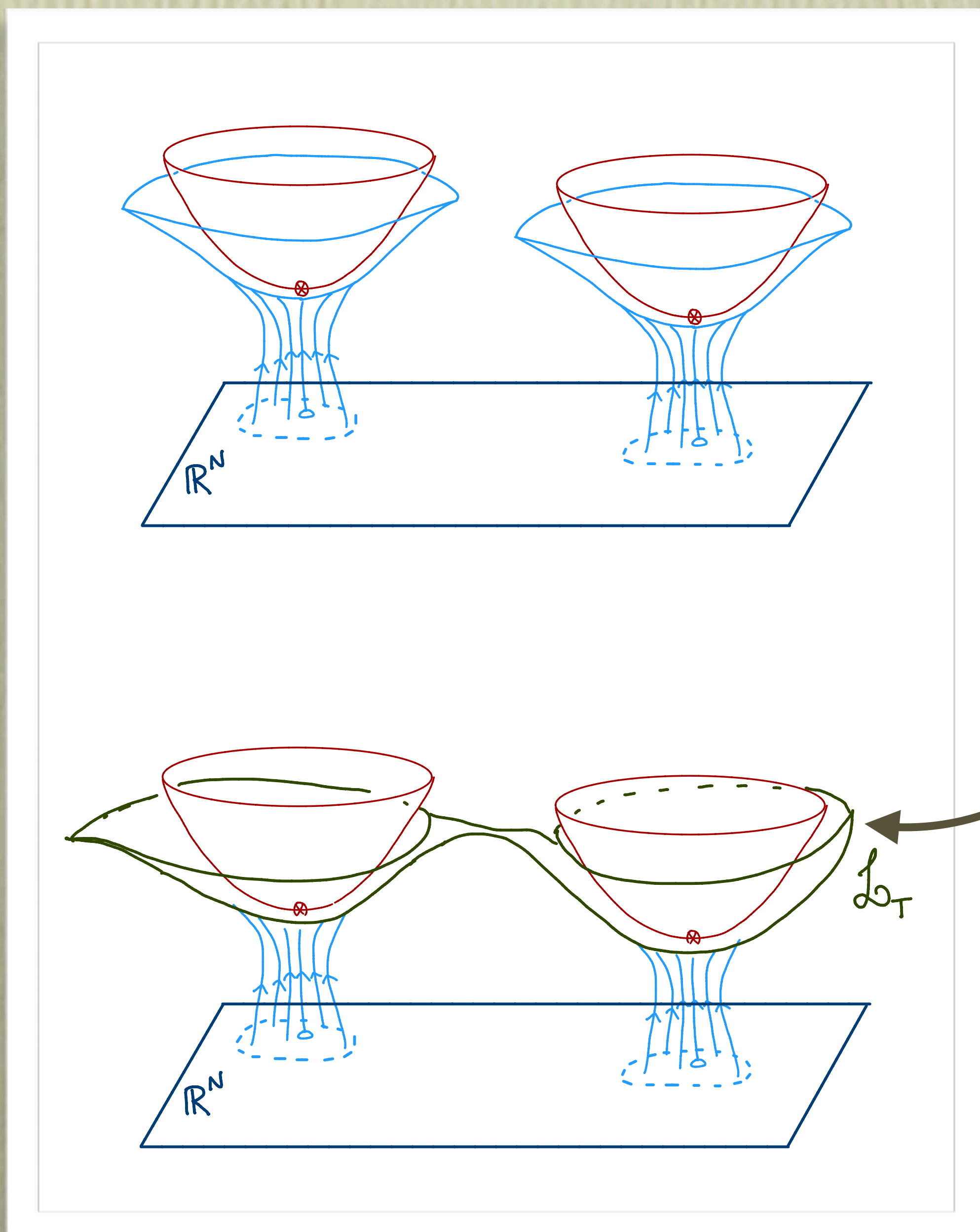
$$Z = \int_{-\infty}^{\infty} \mathrm{d}x\, e^{-S(x)}$$

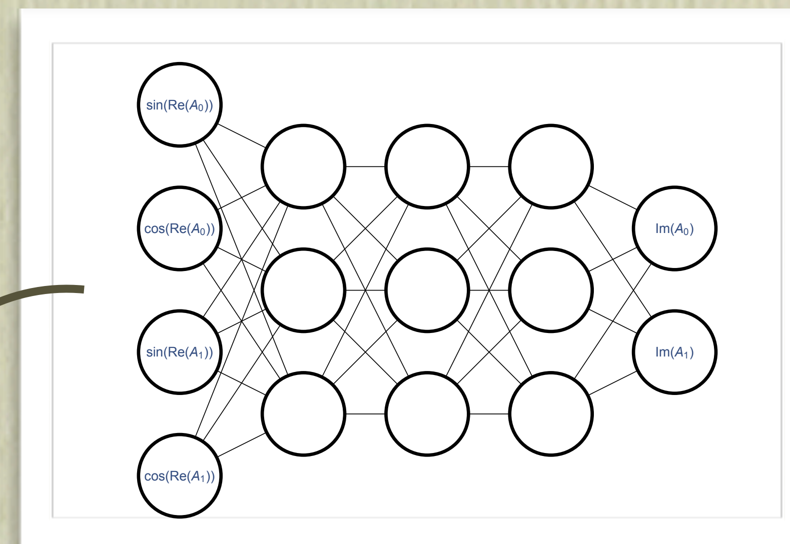
$$S(x) = x^4 - x^2 + 10ix$$

$$Z = \int_{\mathcal{C}} \mathrm{d}z\, e^{-S(z)}$$

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

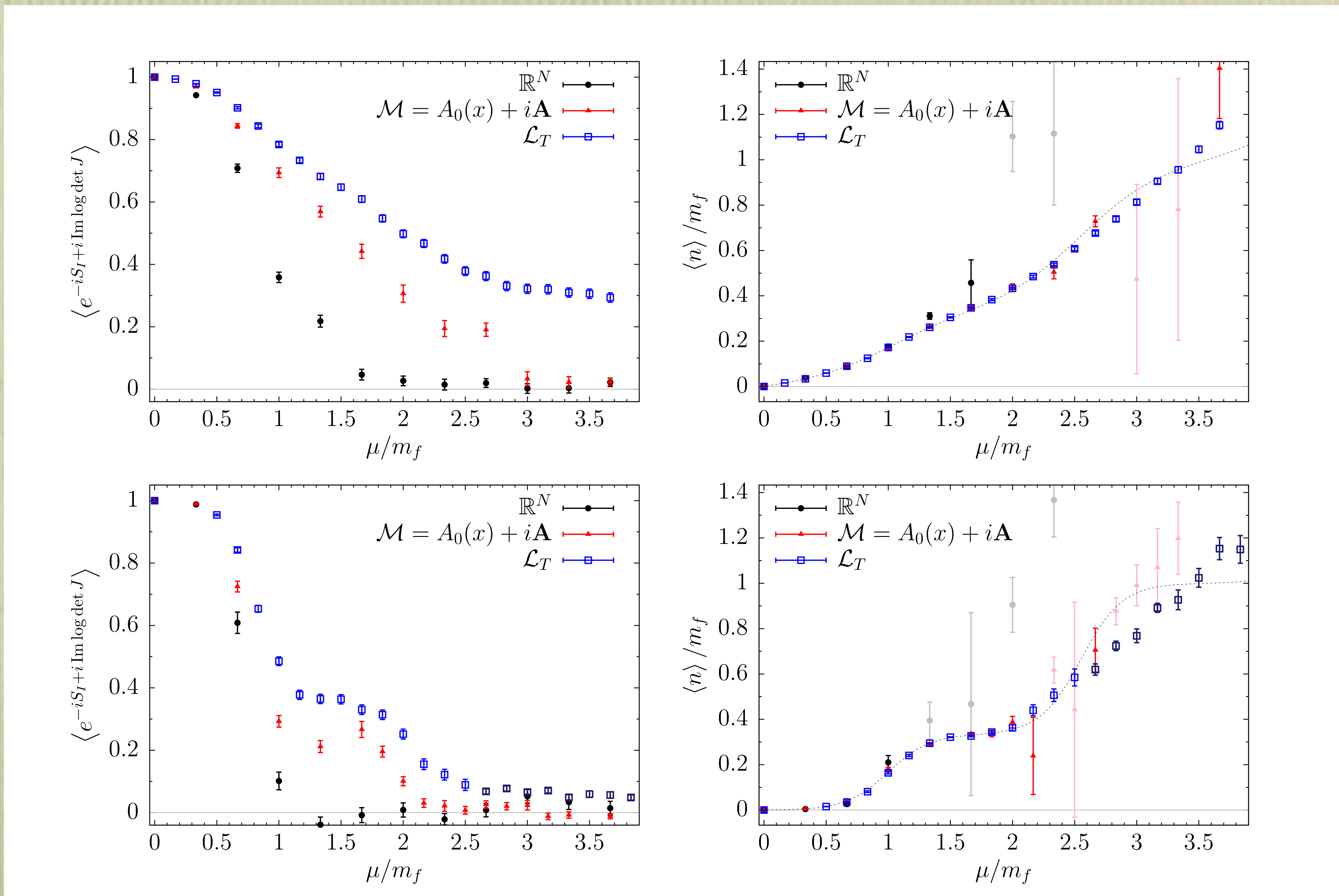
Learnifold





- 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



$\mathbb{R}^N$
$\mathcal{M} = A_0(x) + i\mathbf{A}$
$\mathcal{L}_T$
$\left\langle e^{-iS_I + i\,\mathrm{Im}\log\det J} \right\rangle$
$\langle n \rangle / m_f$
μ / m_f

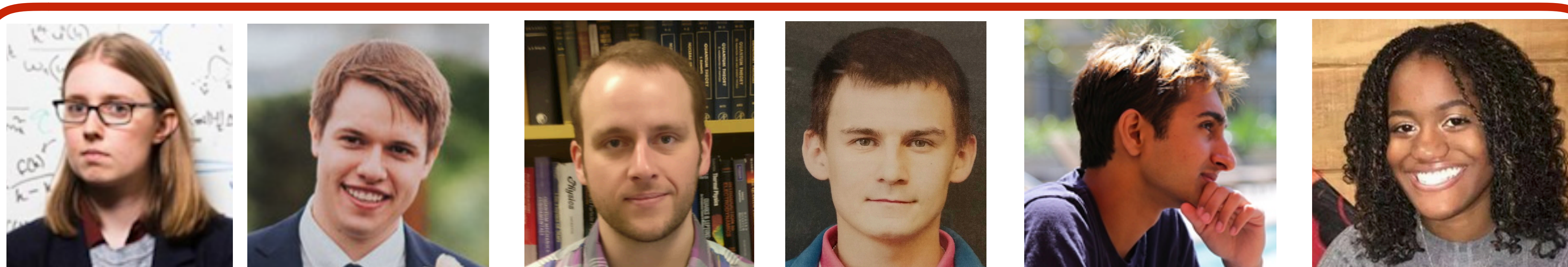
Machine learning QCD

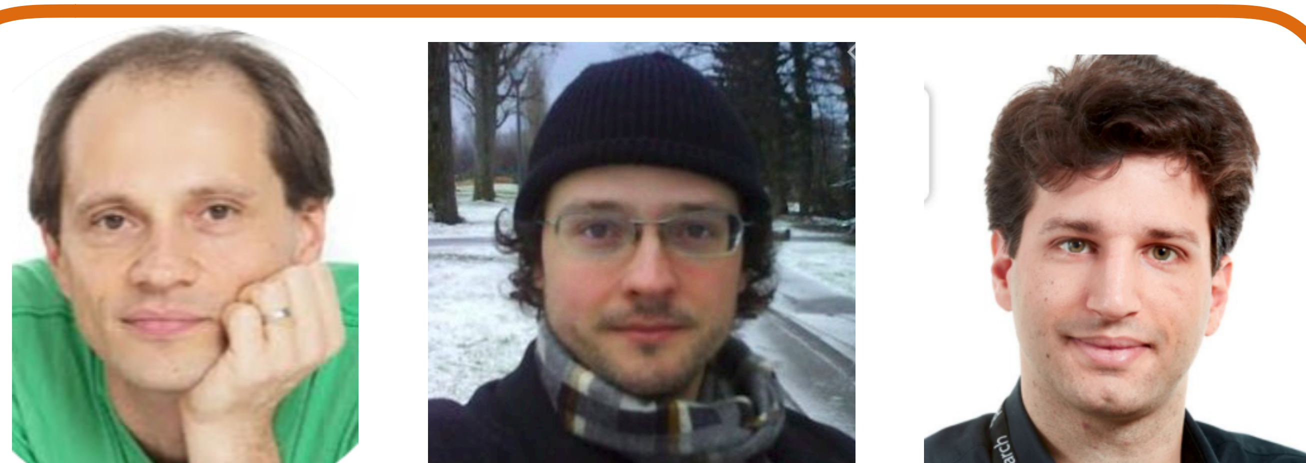
Generative models for QCD gauge field generation

Massachusetts Institute of Technology

Google DeepMind

NYU



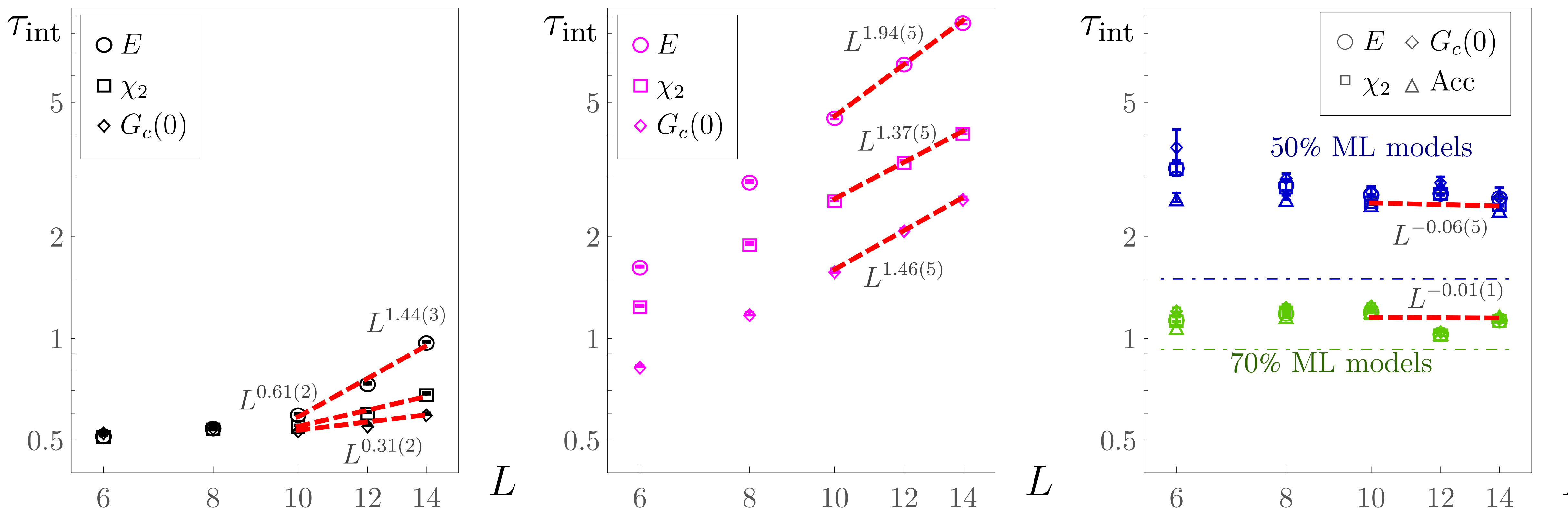


Application: scalar field theory

First application: scalar lattice field theory

Success: Critical slowing down is eliminated

Cost: Up-front training of the model



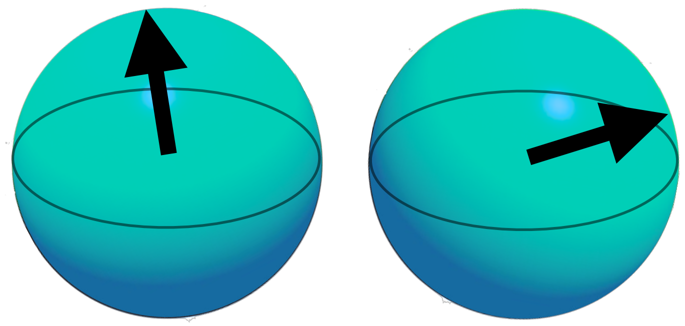
(a) HMC ensembles (b) Local Metropolis ensembles (c) Flow-based MCMC ensembles

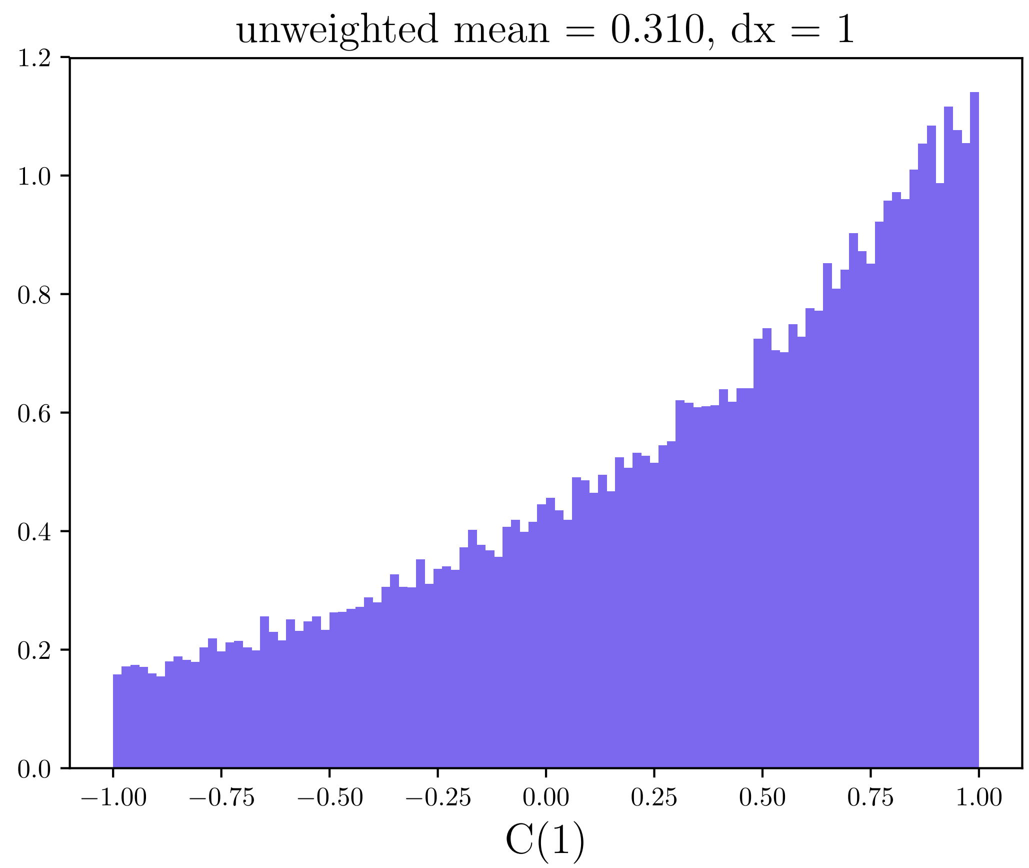
Dynamical critical exponents consistent with zero

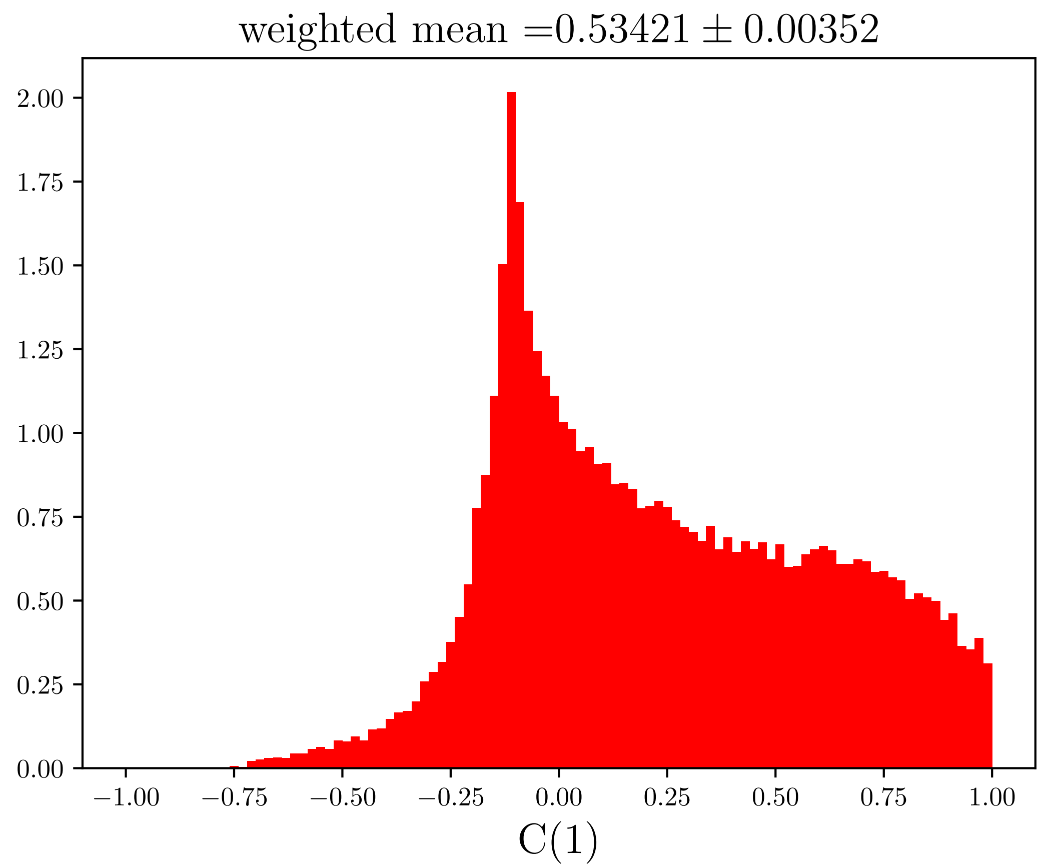
Shanahan: Ensemble generation

Quantitative correlations

$$C(1,\beta = 1) = 0.53731 \qquad \langle \mathcal{O} \rangle = \sum_i \mathcal{O}_i \frac{p_i}{q_i} \Big|_q$$

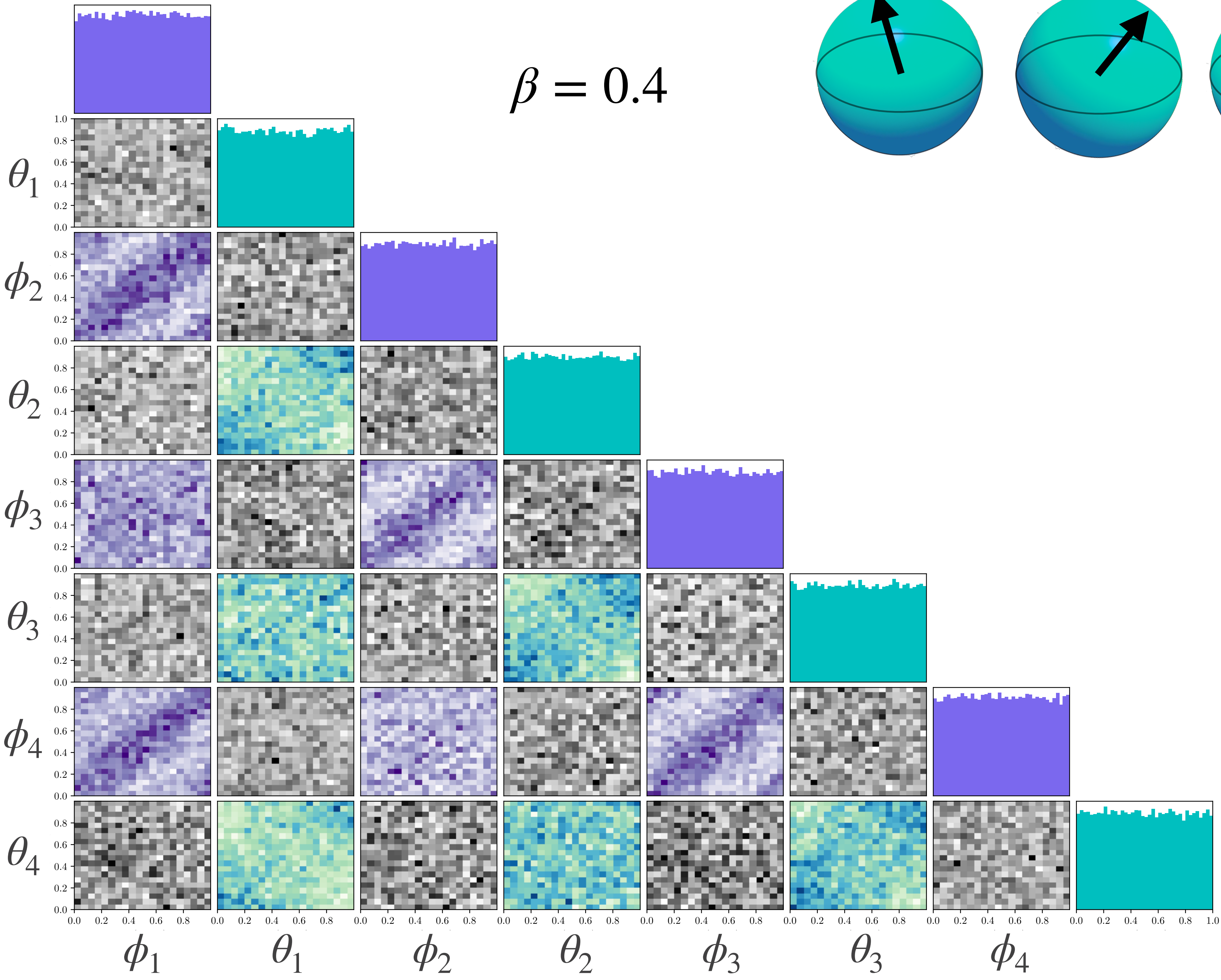


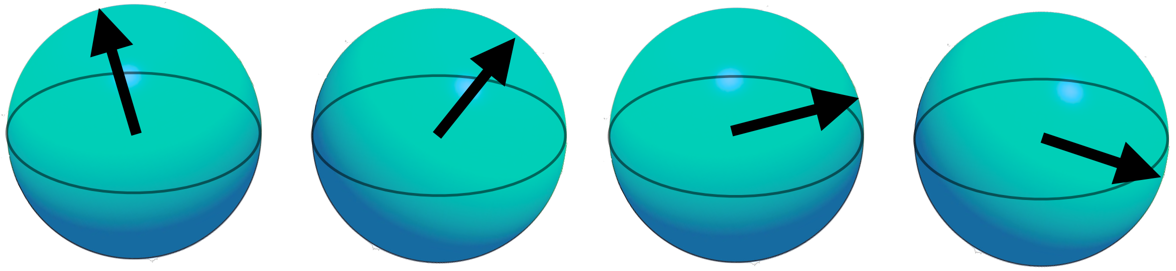




Quantitative correlations

$\beta = 0.4$





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 facutly 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)