

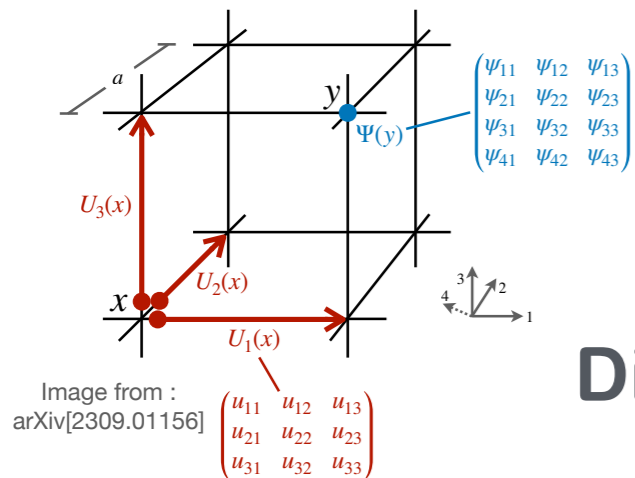
ML Unfolding for error reduction in Lattice QCD observables

EuCAIFCon 2024

1st May 2024

Poster # 77
Thu : 12-15

Simran Singh - Postdoc @ Bielefeld LGT group



Lattice QCD - currently our best probe for understanding **low energy QCD**

Discretise space-time and move to Euclidean space



Sample Gauge configurations from a probability distribution



$$Z = \int \mathcal{D}U \det M_f^n e^{-S_G}$$

Compute observables on the generated configurations $\mathcal{O}(\sim (1 - 10)K)$

$$\langle \mathcal{O} \rangle \sim \frac{\partial \ln Z}{\partial K} \sim \text{Tr} \left(M_f^{-1} \frac{\partial M_f}{\partial K} \right)$$

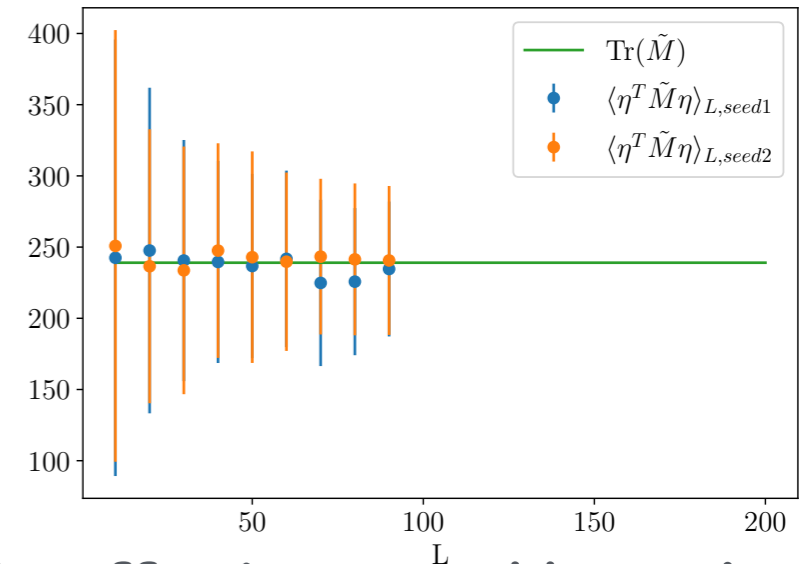
Typical size of Fermion matrices : $N_\sigma^3 \times N_\tau \times N_c \times 4$, can go up to $\sim O(10^7 - 10^9)$

Random Noise Method

No access to individual matrix elements - only matrix vector products !

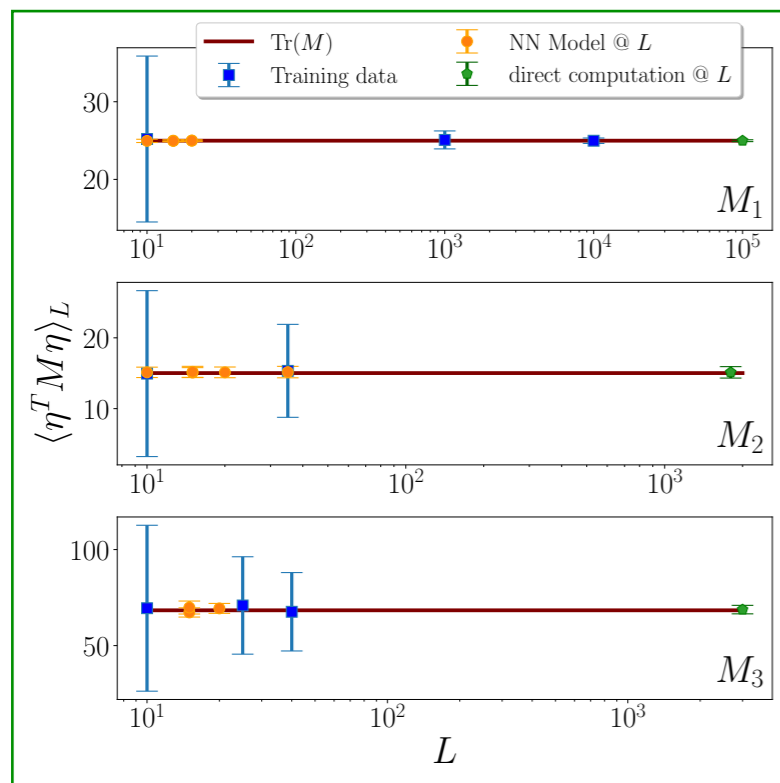
Choose L randomly drawn vectors η satisfying certain conditions to get

$$\langle \eta^T M \eta \rangle_L \simeq \text{Tr} M + \mathcal{O} \left(\frac{f(M)}{\sqrt{L}} \right)$$



Data Unfolding via NN

Question 1 : Can we train a **NN** to learn the systematic effect caused by using only finite such random vectors - given for some observable the **true distribution** with very large L and **measured distribution** with very small L ?



Question 2 : How does this generalise to different Matrices?

Poster # 77
on Thu !

ML Unfolding for error reduction in Lattice QCD observables
 Simran Singh, Universität Bielefeld, Germany

UNIVERSITÄT BIELEFELD
 Faculty of Physics

Computing observables in lattice QCD

- In lattice QCD, fermions integrated out to give $Z = \int \mathcal{D}U \det M_f^n e^{-S_0}$
- Observables \rightarrow derivatives of $\ln Z$, e.g. quark number density: $\frac{\partial \ln \det M_f}{\partial \mu_f} = \text{Tr} \left(M_f^{-1} \frac{\partial M_f}{\partial \mu_f} \right)$
- Typical size of Fermion matrices: $N_f^2 \times N_s \times N_c \times 4$, can go up to $\sim O(10^7 - 10^9)$
- No direct access to matrix elements, only vector products.

Random Noise method

- Current state of art method to compute these traces based on drawing random vectors from a distribution satisfying $\langle \eta_i \rangle = \lim_{L \rightarrow \infty} \frac{1}{L} \sum_{m=1}^L \eta_i^m = 0$ & $\langle \eta_i \eta_j \rangle = \lim_{L \rightarrow \infty} \frac{1}{L} \sum_{m=1}^L \eta_i^m \eta_j^m = \delta_{ij}$
- Trace of M is then given by: $\langle \eta^T M \eta \rangle_L \simeq \text{Tr} M + \mathcal{O} \left(\frac{f(M)}{\sqrt{L}} \right)$
- Only true in the limit of sampling infinite such randomly drawn vectors.

ML based Unfolding: Try to un-learn the effect of finite # of random sources

- Goal: To reconstruct the underlying "true" distribution from observations, which are smeared by "limited experimental" resolution.
- Equivalent to solving the inverse problem: $F_{\text{observed}}(x) = \int K(x,y) * F_{\text{true}}(y) dy$, with the goal to learn $K^{-1}(x,y)$, given F_{true} & F_{observed}
- Can one adapt this to reduce error on the estimate for $\text{Tr} M$ by asking whether we can train a sequential NN on two distributions: one with very small number of sources F_{observed} and the other with very large number of sources F_{true} ?
- Could we then perform measurements on different matrices with small number of sources and apply this transformation to estimate their true trace?

Results of experiments

- Tests performed on matrices with different structures - sparse and dense, different sizes - 100, 1000, 10000, Poisson and normally distributed elements.
- Re-training has to be done but needs fewer resources!

Re-training on M_1 ($L = 10$ & $L = 10^3$)
 First training on M_1 ($L = 10$ & $L = 10^3$)
 Re-training on M_2 with $L = 10$ & $L = 35$
 Re-training on M_3 with $L = 10$ & $L = \{20, 25\}$

Next step: Apply to real QCD data ...