Scalar Content of Nucleon with the Gradient Flow and Machine Learning

August 4th, 2023 | Giovanni Pederiva, Jangho Kim, Andrea Shindler | Lattice 2023
Calculation of Hadronic Matrix Elements that Couple to Dark Matter

- A weakly interacting massive particle (WIMP) is a very popular dark matter (DM) candidate, with various ongoing experiments around the world provide rather severe constraints for the parameters of the models.
- A WIMP type of DM particles, due to its assumed large mass, produces a Higgs boson that couples to the various quark flavor scalar density operators taken between nucleon states.
- At zero momentum transfer, the cross section for spin independent elastic WIMP–nucleon \( (\chi N) \) scattering reads

\[
\sigma_{\chi N} \sim \left| \sum_f G_f(m_{\chi}^2) f_{T_f} \right|^2 \quad \text{with} \quad f_{T_f} = \frac{m_f}{m_N} \langle N | \bar{q}_f q_f | N \rangle = \frac{m_f}{m_N} g_f^s.
\]
Lattice Calculation

- Lattice QCD determination of the nucleon matrix elements from first principles.
- Direct calculation is numerically very challenging (disconnected diagrams).
- Gradient flow helps to reduce the statistical error.\(^1\)
- The matrix element we are interested in

\[
\begin{align*}
g_\ell^S &= \frac{G_\pi}{G_{\pi,t}} \cdot \left[ \langle \mathcal{N} S^\ell(t) \bar{N} \rangle^{con} + \langle \mathcal{N} S^\ell(t) \bar{N} \rangle^{disc} - \langle S^\ell(t) \rangle \langle \mathcal{N}\bar{N} \rangle \right]. \\
g_s^S &= \frac{G_\pi}{G_{\pi,t}} \cdot \left[ \langle \mathcal{N} S^s(t) \bar{N} \rangle^{disc} - \langle S^s(t) \rangle \langle \mathcal{N}\bar{N} \rangle \right].
\end{align*}
\]

\(^1\)See DOI:10.22323/1.214.0251 and A. Shidler talk from Monday 31/7 for more details.
Numerical Strategy

- We compute the quark disconnected diagrams stochastically using the Hutchinson trace method.

\[
\text{Tr}[A] \approx \frac{1}{N_\xi} \sum_{\xi} z_\xi^\dagger A z_\xi
\]  

(4)

- Here \( z_\xi \) is one of \( \{1, -1, i, -i\} \) as in a \( Z_4 \) random noise source.

- We apply the gradient flow and we define \( A = K(t)SK^\dagger \), where \( K^\dagger \) is the adjoint kernel which flows the source of the propagator \( S \), while \( K \) flows the propagator sink.

- Hence, \( KSK^\dagger = S(t, t) \).

\[
\text{Tr}[S(t)] \approx \frac{1}{N_\xi} \sum_{\xi} z_\xi^\dagger K(t, 0)SK^\dagger(0, t)z_\xi.
\]  

(5)

- The gradient flow has the added benefit of a noise reduction effect.
Signal to Noise Ratio Study

- We combine the disconnected diagram calculation with their respective nucleon-nucleon 2-pt function.
- We study the signal to noise ratio as a function of the number of stochastic sources $N_\xi$ in $N_{src}$ sources stochastic locations for the nucleon 2pt correlator at $t/a^2 = 1$.

As a consequence, we have determined that with $N_\xi \approx 10$ and $N_{src} \approx 20$, the signal to noise ratio is saturated.
Quark Condensate \( S^f(t) = \bar{\chi}^f(t, x) \chi^f(t, x) \)

- Light and strange quark condensates at \( t/a^2 = 0 \).

- Euclidean time independent quantity.

- A huge number of inversions is required: \( N_{src} \times N_{conf} \times N_{flow} \times N_{flavors} \)

- Since they are strongly correlated, we developed a ML method which uses subset of the ensemble and predict the remains.
Correlations in the Training Set

This correlation provides a non-trivial mapping from $S^s(t/a^2 = 0)$ to $S^\ell(t/a^2 = 0)$. 
### Lattice Ensemble and ML Sets

<table>
<thead>
<tr>
<th>Ens</th>
<th>$\beta$</th>
<th>$\kappa_l$</th>
<th>$\kappa_s$</th>
<th>$V$</th>
<th>$m_\pi$ [MeV]</th>
<th>$m_N$ [GeV]</th>
<th>$N_{\text{conf}}$</th>
<th>$a$ [fm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$M_1$</td>
<td>1.90</td>
<td>0.13700</td>
<td>0.1364</td>
<td>$32^3 \times 64$</td>
<td>699.0(3)</td>
<td>1.585(2)</td>
<td>399</td>
<td>0.0907(13)</td>
</tr>
</tbody>
</table>

- light quark condensate $S^\ell(t)$

\[
\begin{array}{cccccccccc}
 t/a^2 & i_{\text{src}} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
 \hline
 0.0 & 50 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 \\
 0.5 & 50 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 \\
 1.0 & 50 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 \\
\end{array}
\]

- strange quark condensate $S^s(t)$

\[
\begin{array}{cccccccccc}
 t/a^2 & i_{\text{src}} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \\
 \hline
 0.0 & 50 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 & 399 \\
\end{array}
\]

- $i_{\text{src}} = 1$ are used for training set.

- test ML method for two cases:
  - Between quark flavors: $S^s(t/a^2 = 0)$ and $S^\ell(t/a^2 = 0)$
  - For different flow time: $S^\ell(t/a^2 = 0.5)$ and $S^\ell(t/a^2 = 1)$
We used Decision Trees with infinite depth for the regression problem, flexible and easy to train (using scikit-learn).

We make use of translation invariance in order to increase the sample of training data in the ML model.

The number of training points: $N_{\text{src}} \times N_{\text{conf}} = 50 \times 64 = 3200$
Deviation: $\Delta S = \frac{|S^{\text{direct}} - S^{\text{DT}}|}{\sqrt{(\delta S^{\text{direct}})^2 + (\delta S^{\text{DT}})^2}}$
Combining with Nucleon 2-point Function

\[ R(y_4, x_4, t) \]
\[ = \frac{\langle N(y_4, 0)|qq^f(x_4, t)|\bar{N}(0, 0) \rangle - \langle qq^f(x_4, t)\rangle\langle N(y_4, 0)\bar{N}(0, 0) \rangle}{\langle N(y_4, 0)\bar{N}(0, 0) \rangle} \frac{G_\pi(0)}{G_\pi(t)} \]
\[ = g_S^f + O(e^{-\Delta E|x_4|}) + O(e^{-\Delta E|y_4-x_4|}) \]

\[ \text{direct} \]

\[ g_S^f(t=0.0) > \]

\[ g_S^f(t=1.0) > \]

Member of the Helmholtz Association August 4th, 2023 Slide 10
Comparison with Direct Calculation

\( g(t = 0.0) > \) direct decision tree

\( g(t = 1.0) > \) direct decision tree 1.35(32)

\( g(t = 0.0) \)  direct-decision tree

\( g(t = 1.0) \)  direct-decision tree
Computing time saving
Calculation of light quark condensate.

<table>
<thead>
<tr>
<th>$t/a^2$</th>
<th>$i_{\text{src}}$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>50</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
</tr>
<tr>
<td>0.1</td>
<td>50</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.2</td>
<td>50</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
</tr>
<tr>
<td>0.3</td>
<td>50</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.4</td>
<td>50</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.5</td>
<td>50</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
</tr>
<tr>
<td>0.6</td>
<td>50</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.7</td>
<td>50</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
</tr>
<tr>
<td>0.8</td>
<td>50</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.9</td>
<td>50</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>1.0</td>
<td>50</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
<td>399</td>
</tr>
</tbody>
</table>

- Full calculation: $399 \times 9 \times 11 \times 2 = 79002$ data points
- Training and input set: $50 \times 11 \times 2 + 399 \times 9 = 4691$ confs
- 5.94% of full calculation is needed for both light and strange quark condensates.
Results of $\sigma_f(t)$ (Preliminary)

- $\sigma_f = m_f g^f_S$
- Input is $g^\ell_S(t = 0.5)$ with 9 stochastic sources.
Light quark connected diagram
Adding light quark connected and disconnected diagrams
Summary and Outlook

- ML can help us reduce the computational cost of computing observables in case of strong correlations.
- We computed $\sigma_s$ terms from disconnected diagram calculations and $\sigma_{\pi N}$ from connected and disconnected contributions.
- Using a machine learning method we achieve similar precision using about 5% of the computing resources compared to direct calculations.
- Need to analyze other ensembles for the continuum limit.
- Other observables (vector, Dslash, tensor) currents instead of scalar are available with the same machine learning method.