Sparsening Algorithm for Multi-Hadron Lattice QCD Correlation Functions

W. Detmold, D.J. Murphy, A. Pochinsky, M. Savage, P. Shanahan, M. Wagman

June 21, 2019

Lattice 2019
Motivation

- Traditionally: gauge cfgs. and propagators expensive, contractions cheap
- More recently, some nuclear physics calculations contraction-dominated
  - Multigrid solvers have accelerated HMC and propagators by $O(10 - 100)$
  - Contraction costs grow exponentially in number of quarks
- Nuclear correlation functions typically computed from “baryon blocks”:
  
  \[ B^{a_1, a_2, a_3}_b (\vec{p}, t; x_0) = \sum_{\vec{x}} e^{i\vec{p} \cdot \vec{x}} \sum_{k=1}^{N_{B(b)}} \tilde{w}_b^{(c_1, c_2, c_3),k} \sum_{i_1, i_2, i_3} \epsilon_{i_1, i_2, i_3} S^{a_1}_{c_{i_1}}(x; x_0) S^{a_2}_{c_{i_2}}(x; x_0) S^{a_3}_{c_{i_3}}(x; x_0) \]

  - Usually many source locations, op. smearings, background fields, etc.
  - FFTs are dominant cost
  - Blocks can be stored and re-used between calculations
- Idea: explore multigrid-like “sparsening” targeting contractions
  - Sparsen at the propagator level and do contractions on coarsened lattice
  - Coarsening spatial directions by $N$ reduces FFT and storage costs by $\sim N^3$
Sparsening

- Prescription: uniformly block spatial directions by a factor $N$, and take first site in each block to define sparsened propagators on coarse lattice
- Distinguish between “full” correlation functions

$$C_{\text{full}} (\vec{p}, t; \vec{x}_0, t_0) = \left\langle 0 \right| \sum_{\vec{x} \in \Lambda_3} e^{i \vec{p} \cdot \vec{x}} \mathcal{O} (\vec{x}, t) \mathcal{O}^\dagger (\vec{x}_0, t_0) \left| 0 \right\rangle$$

$$\Lambda_3 = \{ (n_1, n_2, n_3) \mid 0 \leq n_i < L \}$$

and “sparse” correlation functions

$$C_{\text{sparse}} (\vec{p}, t; \vec{x}_0, t_0) = \left\langle 0 \right| \sum_{\vec{x} \in \tilde{\Lambda}_3 (N)} e^{i \vec{p} \cdot \vec{x}} \mathcal{O} (\vec{x}, t) \mathcal{O}^\dagger (\vec{x}_0, t_0) \left| 0 \right\rangle$$

$$\tilde{\Lambda}_3 (N) = \{ (n_1, n_2, n_3) \mid 0 \leq n_i < L; n_i \equiv 0 \ (\text{mod} \ N) \}$$

- Simple interpretation as modified sink interpolator (partial mom. proj.)
  - Preserves FV spectrum and matrix elements (!)
  - Potentially modifies couplings to excited states, statistical noise, … (?)
- Case study: examine two-point functions and ground state energy extractions on $32^3 \times 48$, $N_f = 3$, $m_\pi \approx 800$ MeV Wilson-clover ensemble
\[ \Gamma(r) = \langle (C(\vec{p}, t; \vec{x}_0, t_0) - \langle C(\vec{p}, t; \vec{x}_0, t_0) \rangle) (C(\vec{p}, t; \vec{x}_1, t_0) - \langle C(\vec{p}, t; \vec{x}_1, t_0) \rangle) \rangle \]

- Relevant scales: \((a \Lambda_{QCD})^{-1} \approx 4.1, (am_\pi)^{-1} \approx 1.7, (a \Lambda_{\chi_{SB}})^{-1} \approx 1.4, \ldots\)
- Block with \(N = 4\) in remainder of talk
Consistency of Two-Point Functions: Early Time

- Sparsened vs. full two-point functions at fixed time separation
- Data has been averaged over source locations

\[
R^2 = 0.82 \\
\text{slope} = 0.95(2) \\
\text{intercept} = 2.2(0.8) \times 10^{-8}
\]

\[
R^2 = 0.52 \\
\text{slope} = 0.97(3) \\
\text{intercept} = 6.3(8.6) \times 10^{-13}
\]
Consistency of Two-Point Functions: Late Time

- Sparsened vs. full two-point functions at fixed time separation
- Data has been averaged over source locations

\[ R^2 = 0.86 \]
\[ \text{slope} = 0.98(2) \]
\[ \text{intercept} = 5.8(6.5) \times 10^{-11} \]

\[ R^2 = 0.41 \]
\[ \text{slope} = 1.09(8) \]
\[ \text{intercept} = -1.2(1.3) \times 10^{-16} \]
Single Hadron Spectrum: Effective Energy Signals

- Full (circles) and sparsened (squares) effective energy signals:

- Correlated ratios:
Single Hadron Spectrum: Nucleon Covariance Matrix

$$\Sigma_{ij} = \left\langle (C_{\alpha}(\vec{p}, t_i) - C(\vec{p}, t_i)) (C_{\alpha}(\vec{p}, t_j) - C(\vec{p}, t_j)) \right\rangle_{\alpha}$$

- Plots show correlation matrix: $$\rho_{ij} = \Sigma_{ij}/\sigma_i\sigma_j$$
- No significant modification to correlations in time direction

$$\kappa(\Sigma) = 5.1 \times 10^7$$

$$\kappa(\Sigma) = 3.2 \times 10^7$$
### Single Hadron Spectrum: Ground State Energy Extraction

- Ground-state energies extracted from correlated, single-exponential fits

\[
f(t; Z_{\text{src}}, Z_{\text{snk}}, E) = \begin{cases} 
    \frac{Z_{\text{src}} Z_{\text{snk}}^*}{2E} \left( e^{-Et} + e^{-E(T-t)} \right), & \text{mesons} \\
    \frac{Z_{\text{src}} Z_{\text{snk}}^*}{2E} e^{-Et}, & \text{baryons}
\end{cases}
\]

- No significant effect on extracted ground state energies

| State | $|\vec{n}|^2$ | $aE$ | $\chi^2$/dof | $\kappa(\Sigma)$ | $aE$ | $\chi^2$/dof | $\kappa(\Sigma)$ |
|-------|---------------|-----|-------------|-----------------|-----|-------------|-----------------|
| $\pi$ | 0             | 0.5948(3) | 1.3(7) | $3.8 \times 10^6$ | 0.5947(3) | 1.4(7) | $2.6 \times 10^6$ |
|       | 2             | 0.6537(4) | 1.3(7) | $4.9 \times 10^8$ | 0.6537(4) | 1.9(8) | $8.8 \times 10^7$ |
|       | 4             | 0.7065(4) | 1.2(7) | $7.9 \times 10^8$ | 0.7065(4) | 1.4(7) | $1.7 \times 10^8$ |
| $N$   | 0             | 1.204(2)  | 0.7(7) | $5.1 \times 10^7$ | 1.205(1)  | 0.7(7) | $3.2 \times 10^7$ |
|       | 2             | 1.233(2)  | 0.6(6) | $5.8 \times 10^7$ | 1.234(1)  | 0.2(4) | $3.5 \times 10^7$ |
|       | 4             | 1.260(2)  | 0.6(6) | $6.1 \times 10^7$ | 1.263(2)  | 0.4(5) | $3.8 \times 10^7$ |
Multi-Hadron Spectrum: Effective Energy Signals

- \( R_A(t) = C_A(t)/[C_N(t)]^A t/a \gg 1 \propto \exp(-\Delta E \cdot t), \Delta E \equiv E_A - A \cdot E_N \)
- Full (circles) and sparsened (squares) effective binding energy signals:

- Correlated ratios:
## Multi-Hadron Spectrum: Ground State Energy Extraction

<table>
<thead>
<tr>
<th>State</th>
<th>$aE$</th>
<th>$\chi^2$/dof</th>
<th>$aE$</th>
<th>$\chi^2$/dof</th>
</tr>
</thead>
<tbody>
<tr>
<td>$NN \ (^{1}S_0)$</td>
<td>2.3961(25)</td>
<td>0.41(52)</td>
<td>2.3961(25)</td>
<td>0.35(48)</td>
</tr>
<tr>
<td>$NN \ (^{3}S_1)$</td>
<td>2.3919(25)</td>
<td>0.61(65)</td>
<td>2.3918(25)</td>
<td>0.53(60)</td>
</tr>
<tr>
<td>$^3\text{He}$</td>
<td>3.5726(83)</td>
<td>0.55(74)</td>
<td>3.5726(84)</td>
<td>0.55(72)</td>
</tr>
<tr>
<td>$^4\text{He}$</td>
<td>4.769(29)</td>
<td>0.37(57)</td>
<td>4.766(27)</td>
<td>0.57(72)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>State</th>
<th>$a\Delta E$</th>
<th>$\chi^2$/dof</th>
<th>$a\Delta E$</th>
<th>$\chi^2$/dof</th>
</tr>
</thead>
<tbody>
<tr>
<td>$NN \ (^{1}S_0)$</td>
<td>$-0.0140(18)$</td>
<td>0.46(67)</td>
<td>$-0.0138(18)$</td>
<td>0.53(72)</td>
</tr>
<tr>
<td>$NN \ (^{3}S_1)$</td>
<td>$-0.0180(17)$</td>
<td>0.26(50)</td>
<td>$-0.0180(17)$</td>
<td>0.29(53)</td>
</tr>
<tr>
<td>$^3\text{He}$</td>
<td>$-0.0434(72)$</td>
<td>0.37(67)</td>
<td>$-0.0431(75)$</td>
<td>0.44(74)</td>
</tr>
<tr>
<td>$^4\text{He}$</td>
<td>$-0.055(13)$</td>
<td>0.36(49)</td>
<td>$-0.054(13)$</td>
<td>0.55(67)</td>
</tr>
</tbody>
</table>
Controlling Excited State Effects

- Can modify sparsened estimator to control coupling to excited states:

\[
\tilde{C}(\vec{p}, t) = \frac{1}{N_{\text{sparse}}} \sum_{x_0 \in \Lambda_{\text{sparse}}} C_{\text{sparse}}(\vec{p}, t; x_0) + \frac{1}{N_{\Delta}} \sum_{x_0' \in \Lambda_{\Delta}} (C_{\text{full}}(\vec{p}, t; x_0') - C_{\text{sparse}}(\vec{p}, t; x_0'))
\]

- Similar to all-mode averaging (AMA) technique [Blum et. al., PRD 88, 094503]

- \( \Lambda_{\Delta} \subset \Lambda_{\text{sparse}} \), ideally \( N_{\Delta} \ll N_{\text{sparse}} \)

- Note: in this study sources are densely packed and highly correlated!
Conclusions

- We have explored a cost-reduction algorithm for multi-hadron correlation functions based on sparsening at the propagator level.
- Ground state energies extracted from sparsened and full correlation functions are consistent.
- Excited state effects are modified, but this can be controlled with an AMA-like technique.
- We are now using these ideas in production calculations:
  1. NPLQCD light nuclear spectrum and MEs @ $m_\pi = 170$ MeV: $N = 6 \Rightarrow \sim 100\times$ speed-up!
  2. Coarse all-to-all propagators for spectrum of $SU(2)$ Adjoint theory with one Dirac flavor [A. Grebe, Friday @ 16:10]
- Paper to appear on the arXiv soon....

Thank you!