Error reduction technique using covariant approximation and application to nucleon form factor

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We demonstrate the new class of variance reduction techniques for hadron propagator and nucleon isovector form factor in the realistic lattice of $N_f = 2 + 1$ domain-wall fermion. All-mode averaging (AMA) is one of the powerful tools to reduce the statistical noise effectively for wider varieties of observables compared to existing techniques such as low-mode averaging (LMA). We adopt this technique to hadron two-point functions and three-point functions, and compare with LMA and traditional source-shift method in the same ensembles. We observe AMA is much more cost effective in reducing statistical error for these observables.

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1. Introduction

In order to precisely evaluate non-perturbative quantities in lattice calculation, the reducing noise-to-signal ratio is one of the most important tasks especially for nucleon electric dipole moment \([1, 2]\), the hadronic contribution to muon anomalous magnetic moment \([3, 4]\), nucleon form factors and structure functions \([5]\), \(\eta'\) meson mass and mixing angle \([3]\) and so on. We consider new strategies to effectively increase statistics without generating the new gauge configurations.

Traditionally translational symmetry on the lattice has been used to increase the statistics of correlation function (correlator) of hadron interpolating operator(s). Since correlators for different source locations with the same relative separations between operators are exactly same in the infinite statistics limit for translational invariant action, the average over several source locations can be regarded as several times more statistical samples if correlation among correlators with different source is negligible. In this case, however, the additional computation of conjugate gradient (CG) at each source locations is needed. Low-mode-averaging (LMA) \([7, 8, 9]\) takes advantage of low-(eigen)mode for its dominant observables e.g. pseudoscalar correlator \([7, 8, 9, 10, 11, 12]\), to remove the cost of additional computation of CG. However for the other observables, nucleon propagator or resonance state and heavy mesons, \([13, 14, 15]\) reported that the statistical error reduction in LMA is less significant than pseudoscalar correlator.

Here we examine the different variance reduction techniques from LMA for nucleon correlator and its three-point function. All-mode averaging (AMA) proposed in \([16]\) reduces variance from all-modes, without introducing bias, and thus should serve as a powerful technique to precisely evaluate the observables including highly composite contribution coming from all-modes. In this proceedings, we explain this idea and show the numerical results of hadron spectroscopy and isovector form factors of nucleon in realistic lattice setup.

2. Covariant approximation averaging

The observable \(\mathcal{O}\) is calculated over gauge ensemble \(\{U_1, U_2, \cdots, U_{N_{\text{conf}}}\}\) to obtain the ensemble average;

\[
\langle \mathcal{O} \rangle = \frac{1}{N_{\text{conf}}} \sum_{i=1}^{N_{\text{conf}}} \mathcal{O}[U_i] + O(N^{-1/2}_{\text{conf}}),
\]

where the second term denotes the uncertainty due to finite number of available gauge configurations. Under a transformation \(g \in G\), where \(G\) is a set of symmetry transformations on the lattice, the link variable is transformed as \(U \rightarrow U^g\). Ensemble average of an observable \(\mathcal{O}\) should be covariant,

\[
\langle \mathcal{O}^g[U] \rangle = \langle \mathcal{O}[U^g] \rangle,
\]

in the infinite statistics \(N_{\text{conf}} \rightarrow \infty\). \(\mathcal{O}^g\) is the transformed observables.

Here we introduce the approximation \(\mathcal{O}^{\text{(appx)}}\) which fulfills the following condition:

Appx-1:

\[
r = \frac{\langle \Delta \mathcal{O} \Delta \mathcal{O}^{\text{(appx)}} \rangle}{\sqrt{\langle (\Delta \mathcal{O})^2 \rangle \langle (\Delta \mathcal{O}^{\text{(appx)}})^2 \rangle}} \simeq 1, \quad \langle (\Delta \mathcal{O})^2 \rangle \simeq \langle (\Delta \mathcal{O}^{\text{(appx)}})^2 \rangle,
\]

with \(\Delta X = X - \langle X \rangle\). \(r\) is the correlation between \(\mathcal{O}\) and \(\mathcal{O}^{\text{(appx)}}\).

Appx-2: The computational cost of \(\mathcal{O}^{\text{(appx)}}\) is much smaller than original \(\mathcal{O}\).
Appx-3: Covariance of approximation : \( \langle \theta^{\text{appx}}[U^g] \rangle = \langle \theta^{(\text{appx})}[g[U]] \rangle \).

Using \( \theta^{(\text{appx})} \) we construct improved estimator;

\[
\theta^{(\text{imp})} = \theta^{(\text{rest})} + \theta_G^{(\text{appx})}, \quad \theta^{(\text{rest})} = \theta - \theta^{(\text{appx})}, \quad \theta_G^{(\text{appx})} = N_G^{-1} \sum_{g \in G} \theta^{(\text{appx})} g.
\] (2.4)

The first and the second conditions are to reduce statistical error of \( \theta^{(\text{rest})} \) and the computational cost respectively at fixed \( N_{\text{conf}} \), while the third one is to avoid the bias : it leads to \( \langle \theta^{(\text{imp})} \rangle = \langle \theta \rangle \).

When we perform \( N_G \) times measurements for \( \theta^{(\text{appx})} \) after transformation \( g \in G \), for instance, shifting source locations, the statistical error of improved estimator, \( \Delta_{\text{(imp)}} \), will be reduced to

\[
\Delta_{\text{(imp)}} \simeq \Delta \sqrt{2(1 - r) + N_G^{-1}},
\] (2.5)

compared with original error \( \Delta \) ignoring the correlation among \( \theta^{(\text{appx})} g \) with different \( g \)’s. In the case of strong correlation, \( r \simeq 1 \), in Appx-1, \( \Delta_{\text{(imp)}} \) becomes nearly \( N_G^{-1/2} \) times smaller than \( \Delta \).

If \( \text{Cost}(\theta^{(\text{appx})}) \) is significantly cheaper than \( N_G \times \text{Cost}(\theta) \) (Appx-2), total cost of \( \theta^{(\text{imp})} \) for a fixed size of error is reduced by a factor \( \simeq \text{Cost}(\theta^{(\text{appx})}) / \text{Cost}(\theta) + N_G^{-1} \) (the last factor comes from computation of \( \theta \) in \( \theta^{(\text{rest})} \)). The above improved estimator defines covariant approximation averaging (CAA).

LMA \([8, 9]\) is one of CAA; \( \theta^{(\text{appx})} \) consists of low-mode, and \( g \) is a shift of source location. In LMA, \( \theta^{(\text{appx})} \) is correlator constructed from a few low-modes of Hermitian Dirac operator \( H(x,y) \) (or its even-odd preconditioned counterpart), where we only present formula for the point source case for simplicity,

\[
S^{(\text{low})}(x,y) = \sum_{k=1}^{N_G} \lambda_k^{-1} \psi_k(x) \psi_k^*(y), \quad \theta_G^{(\text{LMA})} = \frac{1}{N_G} \sum_{g \in G} \theta(S^{(\text{low})} g),
\] (2.6)

with eigenmode \( \psi_k \) and eigenvalue \( \lambda_k \) in \( \sum \psi_k(x) \psi_k^*(y) = \lambda_k \psi_k(x) \). Appx-3 is satisfied since \( \psi_k(x) \) respects the translational symmetry. Cost of \( \theta^{(\text{appx})} \) includes the I/O for eigenmode, outer products of eigenvectors in Eq. (2.5), and the cost to construct quark propagators for \( \theta(S^{(\text{low})}) \), which is typically small cost (Appx-2). Appx-2,3 are satisfied for most of observables in LMA, however, Appx-1 strongly depends on \( \theta \) and size of \( N_k \sim O(100) \).

We proposed another example of CAA, which we call as all-mode averaging (AMA) in \([4]\). Using the sloppy CG \([17]\) combined with low-mode deflation (e.g. \([13]\)) in which the stopping condition \( \epsilon \) of CG is made loose as \( \epsilon_{\text{AMA}} < 10^{-3} - 10^{-4} \) (or fix the number of CG iterations to some small number \(^1\)), the approximation is given by

\[
S^{(\text{all})}(x,y) = \sum_{k=1}^{N_G} \lambda_k^{-1} \psi_k(x) \psi_k^*(y) + f_k(H(x,y)), \quad \theta_G^{(\text{AMA})} = \frac{1}{N_G} \sum_{g \in G} \theta(S^{(\text{all})} g),
\] (2.7)

\(^1\)With the fixed stopping condition of CG in the approximation, \( S^{(\text{all})} \), a bias will be introduced due to the finite precision (64 bits arithmetic in our case) breaking Appx-3 in theoretically very small provability. This bias could be avoided by fixing the iteration number to a constant as pointed out by M. Lüscher and S. Hashimoto independently. In this proceedings, however, we checked that this bias is undetectable by comparing results of AMA and LMA, latter of which does not have such bias: for pion propagator they are identical within 1-\( \sigma \) (0.1\%) error, as shown in Figure \([4]\).
Table 1: Parameters in LMA/AMA. Ranges of CG iteration numbers in each ensembles are shown.

| m  | N_{\text{conf}} | N_G | N_\lambda | \varepsilon | CG iter. | \varepsilon_{\text{AMA}} | CG iter.(AMA) |
|----|------------------|-----|------------|-------------|----------|---------------------|--------------|
| 0.005 | 380 | 32 | 400 | 10^{-8} | 350–360 | 3 \times 10^{-3} | 70–90 |
| 0.01 | 257 | 32 | 180 | 10^{-8} | 600–630 | 3 \times 10^{-3} | 90–130 |

where $f_\varepsilon$ denotes the polynomial function of $H$ implicitly created in CG process to approximate inverse: $f_\varepsilon(\lambda) \sim 1/\lambda$ for $\lambda_N < \lambda < \lambda_{\text{max}}$. AMA has advantage that $s^{(\text{all})}(x,y)$ takes account of not only low-mode contribution but also (approximately) all-mode contribution which is controlled by the two parameters $N_\lambda$ and $\varepsilon_{\text{AMA}}$. AMA also fulfills the above three conditions (Appx-1–Appx-3) for a much wider class of observables than LMA.

3. Numerical results

We use the $N_f = 2+1$ domain-wall fermion (DWF) configurations generated by RBC/UKQCD collaboration in $24^3 \times 64$ lattice at $\beta = 2.13$ Iwasaki gauge action [18]. CG algorithm with four dimensional even-odd preconditioning was used to compute quark propagators at quark mass $m = 0.01, 0.005$, and 5th dimension size is $L_s = 16$. To calculate eigenmode of Hermitian even-odd preconditioned kernel of DWF operator in $10^{-8}$ accuracy, we implement the implicitly restarted Lanczos algorithm with Chebychev polynomial acceleration [19]. Note that in use of even-odd bases, one needs to choose the four dimensional shift vector of source point to meet Appx-3 (even steps in four directions are sufficient).

In this proceedings, LMA/AMA estimator is obtained from $\mathcal{O}^{(\text{appx})}_G$ with $N_G = 32$ different source locations separated by every 12 for spatial direction and 16 for temporal direction; $(0,0,0,0), (12,0,0,0), (12,12,0,0), \cdots, (12,12,12,48)$ in lattice unit. $(0,0,0,0)$ is the original source location for $\mathcal{O}$. Stopping condition $\varepsilon$ for original observable $\mathcal{O}$, and $\varepsilon_{\text{AMA}}$ for the sloppy CG in AMA, are defined as $||Hx - b||/||b|| < \varepsilon,\varepsilon_{\text{AMA}}$ with the even-site source vector $b$ and the even-site solution vector $x$ (see also Table 1). Note that the number of CG iterations is for the case of deflated CG with $N_\lambda$ low-modes. To compare the performance, we set the Gaussian-type smearing source with parameters taken from [5]. In Ref. [5] they measured three- and two-point functions for four source locations in temporal direction to extract the nucleon isovector form factor (and axial charge), and thus $4 \times N_{\text{conf}}$ samples were accumulated. For $m = 0.005$, they have shown the results with quark sources set in two timeslices per one CG (double source method), by which effective samples are doubled. Furthermore their nucleon source was non-relativistic definition (2 spinor sources rather than 4). In our cost analysis below, we will correct these two factors for fair comparison.

3.1 Two-point function

In Figure 1 we compare nucleon ($N$), pseudoscalar ($P$) and vector ($V$) meson correlator on three different time separations for original and LMA/AMA analysis. As mentioned before, LMA suppresses fluctuation from low-modes of Dirac matrix in Eq.(2.6) by averaging over $N_G$ source locations of low-modes, and thus the error reduction of LMA is significant for larger time separations. On the other hand, since AMA approximately averages contribution from all modes, AMA
Figure 1: The comparison between LMA/AMA and original analysis for nucleon (N), pseudoscalar (P) and vector (V) meson propagator at different time-slices $t = 4, 8, 12$. The colored bar indicates the ratio of relative error between original and LMA/AMA. This is the case at $m = 0.005$.

Table 2: The nucleon mass obtained by global fitting of N correlator with Gaussian smeared sink. We use GeV unit. Last two columns are the gain for AMA with and without deflation, which are inverse of reductions of costs to achieve the same size of errors. For Gain$_{w/\text{def}}$, the cost for computing eigenvectors are ignored while Gain$_{w/\text{odef}}$ reflects its cost, see [16] for more detail breakup of costs. Costs of TY [5] are estimated in case of the relativistic source on a single time-slice per a CG for the fair comparison; 1864 meas. ($m = 0.005$) and 1424 meas. in $m = 0.01$.

| $m_\pi$ | $m_N^{\text{Orig}}$ | $m_N^{\text{LMA}}$ | $m_N^{\text{AMA}}$ | $m_N^{\text{TY}}$ | Gain$_{w/\text{def}}$ | Gain$_{w/\text{odef}}$ |
|---------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| 0.33    | 1.124(22)           | 1.145(9)            | 1.139(4)            | 1.148(10)           | 4                   | 15                  |
| 0.42    | 1.221(17)           | 1.219(11)           | 1.233(4)            | 1.217(9)            | 4                   | 5                   |

is expected to suppress the fluctuation of observables in both short and long distances. The above expectation is clearly seen in Figure 1: as a time-separation changes from $t = 12$ to $t = 4$, the error reduction ratio (green bar) is degraded in LMA significantly, while, for AMA, error reduction rate remains close to the ideal magnitude, $1/N^{1/2} \simeq 0.18$, and always smaller than that of LMA, for every channels and distances. Error reduction for $P$ channel is less different between LMA and AMA. This is likely because the single pion is mostly dominated by the low-modes, also discussed in [7, 8, 9].

In Figure 2, the effective mass of nucleon in AMA becomes flatter for both point and Gaussian smeared sinks compared to those of LMA. In Table 2 we see that the precision of nucleon mass in AMA is higher than previous study [5] while the computational cost is roughly less by 1/4 times. The detailed comparison between them including computational time of low-mode is discussed in [16].
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Figure 2: Effective mass plot of nucleon correlator in original, LMA/AMA analysis with point sink and Gaussian smeared sink. The colored bound shows the statistical error when globally fitting the propagator.

Figure 3: Isovector form factor $F_1(q^2)$ and $F_2(q^2)$ obtained in LMA/AMA and presented in TY et al. at $m = 0.005$. The bars denote the relative error for each $q^2$ results.

3.2 Nucleon isovector form factor

To test AMA for more involved observables, we compare the three-point functions from AMA/LMA with parameters shown in Table 1 and the previous result in [5]. Nucleon isovector form factors, which are particularly feasible test bed, are extracted from the ratio of three and two point functions:

$$R_{\mu}(t_1,t_0|p_1,p_0) = K \frac{C^N_{\mu}(\bar{q},t)}{C^N_G(t_1-t_0,0)} \left[ \frac{C^N_L(t_1-t_0,\bar{q})C^N_G(t-t_0,0)C^N_L(t_1-t_0,0)}{C^N_L(t_1-t_0,\bar{q})C^N_G(t-t_0,0)C^N_L(t_1-t_0,\bar{q})} \right]^{1/2}. \quad (3.1)$$

Here $C^N_{L,G}(t,\bar{q})$ is the two-point function of nucleon with local (L) or Gaussian (G) sink at spatial momentum $\bar{q}$, $C^N_{\mu}(\bar{q},t)$ is the three-point functions with vector current $J_{\mu}$, and $K = \sqrt{2(E_N + m_N)/E_N}$. See [5] for more details. Isovector form factors extracted from Eq. (3.1) are shown in Figure 3. Precision of $F_{1,2}(q^2)$ in AMA is better than the previous results [5] at all transfer momenta $q^2$ examined. This demonstrates that AMA is effective to reduce errors for many lattice observables.
4. Summary

In this proceedings, we have shown several results using the new class of (bias-free) error reduction techniques called as covariant approximation averaging (CAA). We proposed all-mode-averaging (AMA), in which contributions from all eigen modes are taken into account in the averaged approximation with the sloppy CG using deflation. AMA is applicable to a broad variety of observables including nucleon spectrum, three-point functions and other composite correlators. We compared the nucleon mass and isovector form factors for realistic $N_f = 2 + 1$ DWF configurations with lattice volume (2.7 fm$^3$) and light quark masses ($m_\pi \simeq 0.3$–0.4 GeV). Significant gain in computational cost, up to 15 times is observed when compared with traditional many-source method without the deflation (and 4 times compared with the case with deflation). AMA significantly reduces error for cases in which LMA can not so much. Using this technique, calculations of the nucleon electric dipole moment and the hadronic contributions to the muon g-2 are now underway.

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