Disconnected Loop Noise Methods in Lattice QCD

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A comparison of the noise variance between algorithms for calculating disconnected loop signals in lattice QCD is carried out. The methods considered are the $Z(N)$ noise method and the Volume method. We find that the noise variance is strongly influenced by the Dirac structure of the operator.

1. Introduction and Review

The two most widely used numerical techniques for evaluating disconnected amplitudes are the so-called $Z(N)$ noise and Volume noise methods. Disconnected diagrams are needed in calculations of, e.g., the pi-N sigma term, nucleon quark spin content, and pion-pion coupling. These two methods can be thought of as simply using different noise vectors ($Z(N)$ or $SU(3)$) to evaluate summed, disconnected graph amplitudes. Of course the Volume method is specific to gauge theories because it utilizes Elitzur’s theorem. Volume noises are simply equivalent to performing random $SU(3)$ gauge transformations on the configuration.

There are two sources of noise in the simulation. Given $N$ configurations and $M$ random $Z(N)$ or Volume noises, the final error bar is given by

$$\sigma = \sqrt{\frac{S_{\text{noise}}^2}{NM} + \frac{S_{\text{gauge}}^2}{N}}. \quad (1)$$

The comparison here is between the $Z(N)$ and Volume values of $S_{\text{noise}}^2$ for various lattice operators. Such a comparison does not tell how many configurations are necessary to aquire a signal for a given operator, but instead which method will do the best job for a given amount of computer time.

The $Z(N)$ method is a general technique for inverting matrices, based upon the solution of the system of equations,

$$Mx = b, \quad (2)$$

where $M$ is the $N \times N$ quark matrix, $x$ is the solution vector and $b$ is the noise vector. It has the properties

$$<b_i> = 0, <b_ib_j> = \delta_{ij}, \quad (3)$$

where one is averaging over the noise vectors. Any inverse matrix element, $S_{ij} = M^{-1}_{ij}$, can then be obtained from

$$<b_jx_i> = \sum_k S_{ik} <b_jb_k> = S_{ij}. \quad (4)$$

We consider $Z(N)$ noise here, specifically the $Z(2)$ and $Z(4)$ noises. The reason for considering these two cases is that it is known that the variance of any matrix element is the same for $N \geq 3$, but in general the $N = 2$ and $N \geq 3$ variances are different.

The difference in the variance of a given linear combination

$$\sum_{ji} d_{ji} <b_jx_i> = \sum_{ij} d_{ij} S_{ij}, \quad (5)$$

between $Z(2)$ and $Z(N)$ ($N \geq 3$) is given by

$$Var[Z(2)] - Var[Z(N)] = \frac{1}{L} \sum_{m,n,p,r; n \neq r} d_{nm}^T S_{mr}d_{rp}^T S_{pn}. \quad (6)$$

$L$ is the number of noise vectors.) We have been able to find only a single local operator $\bar{\psi}(x)C\psi(x)$ ($C$ is the charge conjugation matrix; $C = \gamma_2$ here) for which the sign of the right-hand side of Eq.(6) can be predicted, implying that $Z(2)$ variance is smaller than $Z(N)$. However, we can not say how large this difference is and a numerical simulation is needed.
An important issue in calculating the noise variance for the Volume method is the generation of random SU(3) matrices. This can be done by calculating the Haar measure for some given parametrization, but there is a simpler way. Consider the mod of SU(3) by a copy of SU(2):
\[
SU(3) \rightarrow \frac{SU(3)}{SU(2)} \sim \frac{SO(6)}{SO(5)} \sim S^5, \tag{7}
\]

The coset space thus consists of all points on a 5-sphere in 6 dimensions and the manifold of SU(3) can be taken to be a 3-sphere (the SU(2) part) times a 5-sphere, giving 5+3=8 real parameters. This gives a particularly easy way of generating random SU(3) matrices. After establishing the relationship between the 5-sphere manifold and the SU(3) parameter space, one need only choose random points on the spheres to generate randomly distributed SU(3) matrices. We have found a parametrization that holds everywhere on the 5-sphere except on a set of measure zero, namely a circle.

Another important issue is the fact that noise methods can be implemented by smearing over different subspaces. For example, the Volume method is usually implemented by smearing over space-time only, which means that \(3 \times 4 = 12\) inverses are necessary to extract a complete column. (One could smear over color indices as well using Elitzur’s theorem, but we find no computational advantage to doing so.) One can implement the \(Z(N)\) noise also with various smearings. The most common is to smear over all indices, resulting in a complete column after a single inversion. We will refer to a method which requires 12 input noise vectors to give a single column as a “12 noise method”, and a method which needs only a single noise vector as a “1 noise method”.

In carrying out our comparisons we consider all local operators, \(\bar{\psi}(x)\Gamma\psi(x)\), as well as point-split versions of the vector and axial vector operators. For each operator there are both real and imaginary parts, but the quark propagator identity \(S = \gamma_5 S^\dagger \gamma_5\), means that only the real or the imaginary part of each local or nonlocal operator is nonzero on a given configuration. Our operators are (averaged over all space-time points):

**Scalar:** \(\text{Re}[\bar{\psi}(x)\psi(x)]\),

**Local Vector:** \(\text{Im}[\bar{\psi}(x)\gamma_\mu \psi(x)]\),

**P-S Vector:** \(\kappa \text{Im}(\bar{\psi}(x+a_\mu)(1+\gamma_\mu U_\mu)(x)\psi(x) - \bar{\psi}(x)(1-\gamma_\mu U_\mu(x)\psi(x+a_\mu))\),

**Pseudoscalar:** \(\text{Re}[\bar{\psi}(x)\gamma_5 \psi(x)]\),

**Local Axial:** \(\text{Re}[\bar{\psi}(x)\gamma_5 \gamma_\mu \psi(x)]\),

**P-S Axial:** \(\kappa \text{Re}[\bar{\psi}(x+a_\mu)\gamma_5 \gamma_\mu U_\mu^\dagger(x)\psi(x) + \bar{\psi}(x)\gamma_5 \gamma_\mu U_\mu(x)\psi(x+a_\mu)]\),

**Tensor:** \(\text{Im}[\bar{\psi}(x)\sigma_{\mu\nu} \psi(x)]\).

### 2. Results and Conclusions

The sample variance in \(M\) quantities \(x_i\) is given by the standard expression:
\[
S_{\text{noise}}^2 = \frac{1}{M-1} \sum_{i=1}^{M} (x_i - \bar{x})^2. \tag{8}
\]

What we concentrate on here are the relative variances between the different methods. Since the square of the noise error is given by \(\sigma_{\text{noise}}^2 = S_{\text{noise}}^2/M\), a ratio of variances (weighted by the number of inverses or noises required) gives a multiplicative measure of the relative efficiency. One important caveat, however. We are doing a fixed number of iterations for all of the operators; it could very well be that different methods will require significantly different numbers of conjugate-gradient iterations to reach the same level of accuracy. For these reasons, we prefer to refer to our results as “pseudo-efficiencies” (“PE”) which are defined by
\[
\text{PE}(\text{method1})/\text{PE}(\text{method2}) = \frac{N_{\text{method1}}(S_{\text{noise1}}^2)}{N_{\text{method2}}(S_{\text{noise2}}^2)}, \tag{9}
\]
where \(N_{\text{method}}\) are the number of noise vectors required to achieve one column of the inverse.

At present, we have results only for one rather small \(\kappa\) value, \(\kappa = 0.148\), using 10 noises on 10 configurations. We look at 4 methods: \(Z(2)\) (1 noise), \(Z(4)\) (1 noise), \(Z(2)\) (12 noise), and Volume (12 noise). Note that no gauge fixing on the configurations was done in the \(Z(N)\) noise cases.

A selection of our numerical results appears in Table 1 where only the pseudoefficiencies of the two 12 noise methods relative to 1 noise \(Z(2)\) is presented. In this table “Local Vector1” means the local operator \(\bar{\psi}(x)\gamma_1 \psi(x)\), “P-S Vector1”
Table 1
Pseudoefficiency ("PE") of 12 noise methods vs. 1 noise Z(2).

| PE(12 noise Volume) vs. 1 noise Z(2) | PE(12 noise Z(2)) |
|-------------------------------------|-------------------|
| **Scalar:**                         | **PE(12 noise Z(2))** |
| 0.121E + 02 ± 0.32E + 01           | 0.109E + 02 ± 0.25E + 01 |
| **Local Vector1:**                  |                   |
| 0.953E + 01 ± 0.21E + 01           | 0.871E + 01 ± 0.18E + 01 |
| **Local Vector2:**                  |                   |
| 0.118E + 02 ± 0.16E + 01           | 0.121E + 02 ± 0.29E + 01 |
| **Local Vector3:**                  |                   |
| 0.958E + 01 ± 0.25E + 01           | 0.114E + 02 ± 0.24E + 01 |
| **Local Vector4:**                  |                   |
| 0.137E + 02 ± 0.32E + 01           | 0.163E + 02 ± 0.34E + 01 |
| **P-S Vector1:**                   |                   |
| 0.121E + 02 ± 0.30E + 01           | 0.994E + 01 ± 0.22E + 01 |
| **P-S Vector2:**                   |                   |
| 0.127E + 02 ± 0.21E + 01           | 0.110E + 02 ± 0.23E + 01 |
| **P-S Vector3:**                   |                   |
| 0.968E + 01 ± 0.16E + 01           | 0.114E + 02 ± 0.15E + 01 |
| **P-S Vector4:**                   |                   |
| 0.150E + 02 ± 0.32E + 01           | 0.155E + 02 ± 0.42E + 01 |
| **Pseudoscalar:**                  |                   |
| 0.142E - 01 ± 0.34E - 02           | 0.201E - 01 ± 0.43E - 02 |
| **Local Axial1:**                  |                   |
| 0.162E + 00 ± 0.30E - 01           | 0.144E + 00 ± 0.29E - 01 |
| **Local Axial2:**                  |                   |
| 0.178E + 00 ± 0.45E - 01           | 0.146E + 00 ± 0.37E - 01 |
| **Local Axial3:**                  |                   |
| 0.155E + 00 ± 0.43E - 01           | 0.162E + 00 ± 0.38E - 01 |
| **Local Axial4:**                  |                   |
| 0.204E + 00 ± 0.41E - 01           | 0.187E + 00 ± 0.35E - 01 |
| **P-S Axial1:**                    |                   |
| 0.183E + 00 ± 0.31E - 01           | 0.151E + 00 ± 0.18E - 01 |
| **P-S Axial2:**                    |                   |
| 0.142E + 00 ± 0.29E - 01           | 0.114E + 00 ± 0.28E - 01 |
| **P-S Axial3:**                    |                   |
| 0.197E + 00 ± 0.60E - 01           | 0.186E + 00 ± 0.49E - 01 |
| **P-S Axial4:**                    |                   |
| 0.224E + 00 ± 0.44E - 01           | 0.238E + 00 ± 0.36E - 01 |
| **Tensor41:**                      |                   |
| 0.287E + 00 ± 0.50E - 01           | 0.295E + 00 ± 0.49E - 01 |
| **Tensor42:**                      |                   |
| 0.128E + 00 ± 0.26E - 01           | 0.889E - 01 ± 0.11E - 01 |
| **Tensor43:**                      |                   |
| 0.327E + 00 ± 0.91E - 01           | 0.398E + 00 ± 0.13E + 00 |
| **Tensor12:**                      |                   |
| 0.471E + 00 ± 0.64E - 01           | 0.376E + 00 ± 0.66E - 01 |
| **Tensor13:**                      |                   |
| 0.477E + 00 ± 0.14E + 00           | 0.363E + 00 ± 0.53E - 01 |
| **Tensor23:**                      |                   |
| 0.562E - 01 ± 0.91E - 02           | 0.751E - 01 ± 0.16E - 01 |

means the point-split version, and the local operator $\bar{\psi}(x)\gamma_4\gamma_1\psi(x)$ is denoted as “Tensor41”, etc. A quick examination of this table reveals that there are large and dramatic differences in the pseudoefficiencies among the various operators. 1 noise methods are approximately 10 to 15 times more efficient than either 12 noise method for scalar and vector operators; conversely, 12 noise methods are much more efficient for pseudoscalar, axial and tensor operators. The most extreme of the entries is for the pseudoscalar, which is approximately 60 times more efficiently calculated with a 12 noise method than with 1 column Z(2). Although the results are not shown here, we have also found pseudoefficiencies close to unity for 12 noise Volume vs. 12 noise Z(2) or of 1 noise Z(2) vs. 1 noise Z(4).

In conclusion, we have seen that the important distinction is not between Z(N) and Volume methods, but between 12 and 1 noise methods and that the pseudoefficiencies are strongly influenced by the Dirac structure of the operator.

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