Stochastic Estimation with $Z_2$ Noise

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Abstract

We introduce a $Z_2$ noise for the stochastic estimation of matrix inversion and discuss its superiority over other noises including the Gaussian noise. This algorithm is applied to the calculation of quark loops in lattice quantum chromodynamics that involves diagonal and off-diagonal traces of the inverse matrix. We will point out its usefulness in its applications to estimating determinants, eigenvalues, and eigenvectors, as well as its limitations based on the structure of the inverse matrix.
Either formally or as a result of numerical practicality, many physical systems, be they classical or quantum mechanical, are boiled down to solving matrix equations. As the dimension $N \times N$ of the matrix $M$ approaches the limit of solving the matrix equation $MX = S$ computationally for a source $S$ with dimension $N \times 1$, it becomes unfeasible to solve it for an $S$ of dimension $N \times N$ using the same algorithm. This is so simply because it requires $N$ times more computational time as that of solving for a column of $S$. In physics applications, sometimes one needs to compute quantities which amounts to solving for the whole matrix $S$, e.g. calculating the diagonal and off-diagonal traces of $M^{-1}$. This poses a numerical challenge, sometimes a grand one. Especially hard is when the dimension of the matrix $M$ grows fast with the physical variables of the problem. For example, when $M$ is represented in the space-time coordinates, the dimension $N$ grows as $L^4$ where $L$ is the size of the space-time dimension. Quark matrix in lattice gauge calculation of quantum chromodynamics (QCD) falls in this category. A space-time lattice with merely the size of $16^3 \times 24$ gives a quark matrix of the dimension $10^6 \times 10^6$ including the spin and color degrees of freedom. While it is durable to calculate the quark propagator, i.e. $M^{-1}(x,0)$ for a point source $S$ at 0 with a reasonably small quark mass (e.g. a fraction of the strange quark mass) on today’s supercomputers, the quark propagator $M^{-1}(x,y)$ from any point to any point is certainly unattainable. For calculations of the 2-point functions or 3-point functions with direct insertions, one can get by with the help of translational symmetry. But there are cases where one can not rely on such a help. These include the calculations of quark loops which are space-time or space integrations of the fermion propagators. Examples of interest in QCD include the quark condensate and the topological susceptibility with the fermion method [3], flavor-singlet meson masses which involve disconnected quark loops in the two-point functions, notably the $U(1)$ problem., and the $\pi N \sigma$ term and the proton spin problem which involve quark loop contributions in the three-point functions.

Instead of waiting for the advent of more powerful hardware, there have been several suggestions to solve it approximately with the stochastic approach. One is the pseudo-fermion method [1] the other is the stochastic estimation with the Gaussian noise [2]. We shall pursue the avenue of stochastic estimation with various noises to see if one kind of noise is better than the others.

The idea of introducing noises is hardly new in physics. Historically, it was introduced to account for the Brownian motion with the Langevin and Fokker-Planck equations, to compute the time-dependent correlation functions in statistical mechanics [4], for the stochastic formulation of quantum mechanics [5] and quantum field theory [6]. Stochastic approach to estimating the inverse of an $N \times N$ matrix $M$ entails the introduction of an ensemble of $L$ column vectors $\eta \equiv \eta^1, ..., \eta^L$ (each of dimension $N \times 1$) with the properties of a white noise, i.e.

\[
\langle \eta \rangle = 0, \quad \langle \eta_i \eta_j \rangle = \delta_{ij}, \quad (1)
\]

where the stochastic average $\langle \cdots \rangle$ goes over the ensemble of the noise vectors $L$;
e.g. $\langle \eta_i \eta_j \rangle = \frac{1}{L} \sum_{n=1}^{L} \eta_i^n \eta_j^n$ where $\eta_i^n$ is the i-th entry in the noise vector $\eta$.

The expectation value of the matrix element $M_{ij}^{-1}$ can be obtained by solving for $X_i$ in the matrix equations $MX = \eta$ with the L noise vectors $\eta$ and then take the ensemble average with the j-th entry of $\eta$

$$E[M_{ij}^{-1}] = \langle \eta_j X_i \rangle = \sum_k M_{ik}^{-1} \langle \eta_i \eta_k \rangle = M_{ij}^{-1}. \quad (2)$$

which is the matrix element $M_{ij}^{-1}$ itself. The last step was obtained through eq. (1).

The pseudofermion method [1] which is based on the Gaussian distribution yields identical results as the stochastic estimation. But the stochastic algorithm is not limited to the Gaussian noise. Any noise which satisfies eq. (1) will work and one may work better than another. To see how good a noise is, we study the deviations from the orthonormal condition in eq. (1) which is strictly true for $L \to \infty$. For this purpose, we define the following 2 errors for measuring the efficiency of a noise. The first one is the average absolute value of the off-diagonal element and the second is the deviation of the diagonal element from unity

$$C_1 = \frac{1}{N(N-1)} \sum_{i \neq j} | \langle \eta_i \eta_j \rangle |, \quad (3)$$

$$C_2 = \left[ \frac{1}{N} \sum_i (\langle \eta_i \eta_i \rangle - 1)^2 \right]. \quad (4)$$

For large and independent configurations, we expect the central limit theorem to hold, i.e. $C_i \cong \frac{\sigma_i}{\sqrt{L}}$, $i = 1, 2$, where $\sigma_i$ is the standard deviation. We checked and found this relation to hold well for the Gaussian noise, noises with double hump distributions like $\eta^2 e^{-\eta^4/2}$ and $\eta^4 e^{-\eta^{10}/2}$, and the $Z_2$ microcanonical noise $\delta(\eta_x | -1)$ for the dimension $N = 500$. The results of $\sigma_1$ and $\sigma_2$ fitted from the range of $L = 10$ to 150 are given in Table 1.

| noise          | $\sigma_1$ | $\sigma_2$ |
|----------------|------------|------------|
| Gaussian       | 0.78(1)    | 1.49(1)    |
| $\eta^2 e^{-\eta^4/2}$ | 0.79(1)    | 0.43(1)    |
| $\eta^4 e^{-\eta^{10}/2}$ | 0.80(1)    | 0.28(1)    |
| $Z_2$          | 0.77(1)    | 0.00(0)    |

We see from Table 1 that the off-diagonal deviation $\sigma_1$ is about the same for all these noises and is close to the asymptotic value of $\sqrt{2/\pi} [\text{[7]}]$. On the other hand,
the diagonal deviation $\sigma_2$ which depends on the deviation of the higher moment; i.e. $\sigma_2 = \sqrt{\langle \eta^4 \rangle} - 1$ decreases as the distribution tends to the bi-nodal form. It is the largest for the Gaussian case with an asymptotic value of $\sqrt{2}$ and vanishes for the $Z_2$ noise. For this reason, we suspected that the $Z_2$ microcanonical noise may work better than the other noises considered here [8]. In fact, it has been shown recently [9] that the variance of a inverted matrix element due to the stochastic estimation is composed of two parts

$$Var[M_{ij}^{-1}] = \frac{1}{L} \{[M_{ij}^{-1}]^2 C_2^2 + \sum_{k \neq j} [M_{ik}^{-1}]^2 \}. \tag{5}$$

Whereas the second part is independent of the kind of noise used, the first part is proportional to the square of the diagonal error $C_2$ only. Since $Z_2$, or $Z_N$ for that matter, has no diagonal error, i.e. $C_2 = 0$, it produces a minimum variance. Other noises will have larger variances due to the non-vanishing $C_2$. For comparison of different noises, we consider the calculation of chiral condensate which is the trace the inverse quark matrix $M$, i.e. $\langle \bar{\Psi} \Psi \rangle = Tr M^{-1}/V$, for a quenched $16^3 \times 24$ lattice at $\beta = 6.0$ with $\kappa = 0.148$ for the Wilson action. First we used the conjugate gradient program to invert a column of the matrix for a particular gauge configuration and find $\sum_{k \neq 1} [M_{k1}^{-1}]^2/[M_{11}^{-1}]^2 = 0.8$. Assuming this ratio is true for all the other columns based on translational invariance and extending eq. (5) to the variance of the trace, we find that the standard deviation from the $Z_2$ noise is smaller than that from the Gaussian noise by a factor of 1.54. In other words, in order to achieve the same level of accuracy, one would need a Gaussian noise configuration 2.4 times larger than that of the $Z_2$ noise. Since any noise with $C_2 \neq 0$ will need more statistics than the $Z_2$ noise to reach the same accuracy, the $Z_2$ (or $Z_N$) noise is the optimal choice in this sense.

With the error analysis in eq. (5), we now realize where the stochastic inversion algorithm would apply. Since the quark propagator has the generic fall off behavior $e^{-m|x-y|}/(|x-y| + O(a))^n$ (a is the lattice spacing) in the space-time separation with $n = 3$ for short distances, quark loops that involve traces near the diagonal, i.e $|x-y| \sim a$, will have large signals. As long as the far off-diagonal contribution to the variance (the second term in eq. (5)) does not overwhelm the contribution from $[M_{ij}^{-1}]^2$ (the first term in eq. (refeq.variance), the square of the matrix element of interest, the noise to signal ratio will be of the order $1/\sqrt{L}$ for the near-diagonal traces from eq. (5). For the trace itself, there is an extra factor of $1/\sqrt{N}$ due to the translational, gauge and rotational symmetries. This is certainly true for the case when the quark mass $m$ is not very small. For $m \to 0$, it remains to be seen if the inverse power behavior $1/(|x-y| + O(a))^n$ is steep enough to curb the off-diagonal contribution to give a sufficiently small variance for a reasonable $L$. But when one considers the case when $|x-y| >> a$, the signal drops exponentially while the error remains constant. Hence, the noise to signal ratio grows exponentially
and the application of the stochastic method is invalidated under this circumstance. Therefore, one does not expect the stochastic method to be useful for calculating general quark propagators. But it is useful for approximating diagonal and near diagonal traces of the inverse matrix if the inverse matrix itself is dominated by the diagonal and near diagonal terms.

To illustrate how the $Z_2$ noise works in detail, we employ it to invert the quark matrix on a quenched $16^3 \times 24$ lattice at $\beta = 6.0$ for Wilson fermions ($\kappa = .148$) for a particular gauge configuration. We shall report the results of certain diagonal and off-diagonal traces corresponding to the scalar, the pseudoscalar, the vector, and the axial-vector currents. The point-split currents are used for the vector and the axial-vector cases. The accumulated averages for these currents (summed over the spatial points on a time slice) for a gauge configuration are plotted in Fig. 1 against the noise configuration $L$. This shows how they approach the equilibrium up to $L = 200$. Also plotted are the histograms for their distributions. We see that in most cases they do tend to stabilize for $L = 200$. If and when $L = 200$ is sufficient for the purpose of estimating these traces with acceptable errors, this algorithm would save the computing time by a factor of $5838$ as compared to inverting the full matrix (dimension $N = 1.18 \times 10^6$ in this case) with the brute force approach.

The $Z_2$ noise has been employed to calculate quark condensate $\langle \bar{\Psi} \Psi \rangle = Tr M^{-1} / V$ and the topological susceptibility with the fermion method [3], i.e.

$$\chi = \frac{m^2}{V} \langle Tr (\gamma_5 M^{-1}) Tr (\gamma_5 M^{-1}) \rangle.$$ 

The preliminary results [8] give reasonable errors which are a combination of the errors from the stochastic estimation and the gauge configurations. Much like the situation with the glueball masses, we found that the two-point functions for the disconnected quark loops are too noisy due to the exponential fall off of the two-point function $e^{-Mt}$ as a function of $t$. However, the disconnected insertion for the three-point function is different. Since there is only one quark loop correlated with the nucleon propagator say, the situation is not as bad as the two-point function. Preliminary results on the $\pi N \sigma$ term and the flavor-singlet axial charge $g_A^0$ are encouraging [10] and will be reported elsewhere [11].

It is worthwhile noting that the stochastic estimation is particularly successful for the trace (denotes as $\overline{Re \bar{\Psi} \Psi}$ in Fig. 1). As we remarked before, this is due to the translational, color and spin symmetries. As a result, the error is proportional to $1/\sqrt{N}$ where $N$ is the dimension of the matrix. With $N = 1.18 \times 10^6$ in our case and the ratio $\sum_{k \neq 1} |M_{k1}|^2 / |M_{11}|^2 = 0.8$, we predict the error to signal ratio to be $\sqrt{1.5} \times 10^{-3}$ from eq. (4) for $L = 1$. This agrees well with the numerical calculation shown in Fig. 1. Given this level of accuracy, it is feasible to apply the stochastic method to the calculation of the determinant, the eigenvalues, and the eigenvectors of the matrix $M$ which might not be feasible with other algorithms. It is well known that for a Hermitian matrix $M$, the density of states can be written as

$$\rho(\lambda) = -\frac{1}{\pi} \lim_{\varepsilon \to 0} Im Tr G(\lambda + i\varepsilon)$$  (6)
where $G$ is the inverse matrix of $\lambda + i\varepsilon - M$. The determinant of the matrix $M$ can be given as

$$detM = e^{\int \rho(\lambda) \ln \lambda d\lambda}$$

(7)

Since the stochastic method is most successful in estimating the trace of the inverse matrix $M$ for lattice QCD as we have just remarked and it is known that the eigenvalues of $M$ are distributed in a reasonably finite range, it would be worthwhile exploring the possibility that this could be an efficient algorithm for calculating the determinant. Looking for the poles of the density of states in eq. (6) has been frequently used as a way to identify the eigenvalues [12] and the eigenvectors can be obtained from the column of the inverse matrix

$$v_i \sim \lim_{\varepsilon \to 0} \Im G_{ik}(\lambda + i\varepsilon)$$

(8)

for any column $k$ [12].

In conclusion, we have proposed an stochastic algorithm for large matrix inversion with the optimal $Z_2$ noise. We show that it is particularly efficient for estimating traces and near diagonal traces for matrices whose inverses are dominated by the diagonal and near diagonal terms themselves. It is applied to calculate quark loop correlations in the vacuum and disconnected quark loop insertions in the three-point functions in QCD. Noting that it is most successful in estimating traces, we shall explore the feasibility of calculating determinants, eigenvalues, and eigenvectors in the future.

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Figure Caption

Fig. 1 The first and second columns show the accumulated averages of the real and imaginary parts of various current loops as functions of the noise configurations L for a gauge configuration. The third and last columns give the corresponding histograms for their distributions.
