Padé–$Z_2$ stochastic estimator of determinants applied to quark loop expansion of lattice QCD.

J.F. Markham $^a$ T. D. Kieu $^b$

$^a$ School of Physics, University of Melbourne, Vic 3052, Australia
$^b$ CSIRO MST, Private Bag 33, Clayton South MDC, Vic 3169, Australia

We use the Padé–$Z_2$ stochastic estimator for calculating $\text{Tr} \log M$ to compute quark loop corrections to quenched QCD. We examine the main source of error in this technique and look at a way of controlling it.

1. Introduction

In lattice QCD calculation, evaluating the fermion determinant is computationally expensive and as a consequence $\det M$ is often not evaluated and is simply set equal to a constant. This is called the quenched approximation and amounts to neglecting internal fermion loops. The goal of this work is to study the systematic error introduced by quenching and to compensate for quenching errors by constructing an expansion in quark-loop count and using it to improve Monte Carlo estimators of Wilson loops measured on quenched gauge field configurations. We examine a source of statistical error and a method for its partial alleviation.

2. Re-weighting existing quenched QCD configurations

With the full QCD action

$$S[U, \psi, \bar{\psi}] = S_{\text{Wilson}}[U] + S_{\text{gauge}}[U, \psi, \bar{\psi}],$$

the expectation value of some operator, $O$ is given by

$$\langle O \rangle = \frac{1}{Z} \int [dU][d\psi][d\bar{\psi}] O e^{-S[U,\psi,\bar{\psi}]}$$

$$= \frac{1}{Z} \int [dU] O \det M[U] e^{-S_{\text{gauge}}[U]},$$

where

$$Z = \int [dU] \det M[U] e^{-S_{\text{gauge}}[U]}.$$  

By rewriting $S_{\text{Wilson}}[U]$ as

$$-S_{\text{Wilson}}[U] = n_f \log \det M[U]$$

$$= n_f \text{Tr} \log M[U]$$

$$= \delta S[U],$$

and dividing through by $e^{\langle \delta S \rangle}$, (2) becomes

$$\langle O \rangle = \frac{\int [dU] O e^{-S_{\text{gauge}}[U]} e^{(\delta S[U] - \langle \delta S \rangle)}}{\int [dU] e^{-S_{\text{gauge}}[U]} e^{(\delta S[U] - \langle \delta S \rangle)}}.$$  

Expanding the exponential in the fluctuations in $\delta S$ leads to

$$\langle O \rangle = \langle O \rangle_{\delta S=0} + \langle O \delta S \rangle_{\delta S=0} - \langle O \rangle_{\delta S=0} \langle \delta S \rangle_{\delta S=0} + \cdots.$$  

Here, the subscript on $\langle O \rangle_{\delta S=0}$ signifies the quenched expectation value of $O$.

3. Padé–$Z_2$ stochastic estimator for evaluating $\text{Tr} \log M$

In order to make use of (6) one needs to be able to find $\delta S$. We use the Padé–$Z_2$ method to find $\text{Tr} \log M$ as per (6).

The Padé approximant for $\text{Tr} \log M$ can be written as

$$\text{Tr} \log M \approx b_0 \text{Tr} I + \sum_{k=1}^{K} b_k \cdot \text{Tr}(M + c_k I)^{-1}.$$
\[ \text{Tr}(M + c_k I)^{-1} \text{ can be estimated using noise } Z_2 \text{ vectors, } \eta^j. \]

\[ \text{Tr}(M + c_k I)^{-1} \approx \frac{1}{L} \left( \sum_j \eta^j \langle \xi^{k,j} \rangle \right), \tag{8} \]

where \( \xi^{k,j} = (M + c_k I)^{-1}\eta^j \) are the solutions of

\[ (M + c_k I)\xi^{k,j} = \eta^j \tag{9} \]

where \( j = 1, \ldots, L \) and \( k = 1, \ldots, K \). The variance of these estimators can be greatly reduced by subtracting suitably chosen traceless matrices

\[ \text{Tr}(M + c_k I)^{-1} \approx \langle \eta^j ((M + c_k I)^{-1} - P \sum_{p=1}^P \lambda_{p,k} Q^{(p)}) \eta \rangle > \tag{10} \]

where the \( \lambda_{p,k} \) are chosen to minimise the variance of the estimator. The \( Q^{(p)} \) used are

\[ Q^{(p)} = \frac{\eta^p}{(1 + c_k)^{p+1}(D^p - \text{Tr} D^p)}, \]

where \( M = 1 - \kappa D \). The odd powers of \( D \) are traceless, but the even powers greater than two are not. \( \text{Tr} D^4 \) and \( \text{Tr} D^6 \) are calculated from 4 and 6 link loops respectively. For this work we expand to order \( K = 11 \), using \( L = 10 \) noise vectors and \( P = 8 \) traceless subtraction matrices. The variational procedure to set \( \lambda_{p,k} \) was found not to be necessary and so we set them equal to unity. To solve (8) we used the MR\(^3 \) algorithm from [2] and the odd–even preconditioner in from [3].

4. Application to Wilson loops

We apply the preceding numerical techniques to finding improved estimates of Wilson loops. Measurements were made on two sets of \( 10^4 \) gauge field configurations: a set of 103 quenched QCD configurations and a set of 95 full QCD configurations, generated using the MILC collaboration software [4].

Both have \( \beta = 5.436 \), and the full QCD configurations have \( \kappa = 0.16 \) and \( n_f = 2 \). Fig. [4] shows the results for various Wilson loops with corrections done to first order as per (8). In all of Figs. [4] the loop number on the x-axis labels

\[ W_{ij} \text{ from left to right in the following order: } W_{11}, W_{12}, W_{13}, W_{14}, W_{15}, W_{23}, W_{24}, W_{25}, W_{24}, W_{25}, W_{31}, W_{10}, W_{25}. \]

In Figs. [4] and [8] points have been offset slightly for clarity.

5. A method for controlling the statistical error

A method for controlling the statistical error in (11) is suggested by looking at the form of the correlator between the diagonal elements of \( \log M \) and the operator, \( \mathcal{O} \), being measured. Given that \( \mathcal{O} \) and \( \delta S \) can be written

\[ \mathcal{O} = \sum_x O_x, \quad \delta S = \sum_y (\delta S)_y \tag{11} \]

then the first order correction to \( \mathcal{O} \) can be written as

\[ \delta \langle \mathcal{O} \rangle \approx \left\langle \sum_x O_x \sum_y \delta S_y \right\rangle \]
\[ - \left\langle \sum_x O_x \right\rangle \left\langle \sum_y \delta S_y \right\rangle \]
\[ = \sum_{x,y} \left\langle O_x (\delta S_y - \left\langle \delta S_y \right\rangle) \right\rangle \]
\[ = \sum_{x,y} \left\langle O_x \delta \tilde{S}_y \right\rangle \]  
(12)

If we write \( f(r) = \left\langle O_x \delta \tilde{S}_y \right\rangle \), where \( r = |x-y| \), then
\[ \sum_{x,y} \left\langle O_x \delta \tilde{S}_y \right\rangle \rightarrow \int dr d\Omega r^3 f(r) \]  
(13)

Fig. 2 shows \( f(r)/f(0) \) and \( r^3 f(r)/f(0) \) as a function of \( r^2 \) for the case \( O = W_{11} \). The former shows that the two operators are correlated, as would be expected. The latter shows that most of the signal for \( \delta O \) is at small \( r \) and but most of the noise is at large \( r \), and that for large lattices this has the potential to swamp the signal. One way to address the problem is to cut the integral off at some \( r_{max} \).

\[ \left\langle \delta O \right\rangle = \sum_{|x-y| \leq r_{max}} \left\langle O_x \delta \tilde{S}_y \right\rangle \]  
(14)

This has been done using \( r_{max} = 4 \), and the results are shown in Fig. 3. The cut off scheme reduces the size of the statistical error but also loses some signal.

The Monte Carlo estimator for \( \left\langle O \right\rangle \) is
\[ \left\langle \left\langle \delta O \right\rangle \right\rangle = \frac{1}{N} \sum_{n=1}^{N} \sum_{|x-y| \leq r_{max}} O^n_x \delta \tilde{S}_y^n \]  
(15)

An efficient way to do this is with Fourier convolution. Given a windowing function \( W(x-y) \), where
\[ W(x-y) = \begin{cases} 1 & \text{if } |x-y| \leq r \\ 0 & \text{otherwise} \end{cases} \]  
(16)

then (13) becomes
\[ \left\langle \left\langle \delta O \right\rangle \right\rangle = \frac{1}{N} \sum_{n=1}^{N} O^n_x \delta \tilde{S}_y^n W(x,y) \]
\[ = \frac{1}{N} \sum_{n=1}^{N} O^n_x \]
\[ \times \left[ \mathcal{F}^{-1} \left\{ \mathcal{F}[\delta \tilde{S}_y^n] \mathcal{F}[W(x,y)] \right\} \right]_x \]  
(17)

where \( \mathcal{F} \) and \( \mathcal{F}^{-1} \) are defined in the usual way and implemented as fast Fourier transforms. Using this method to compute \( \left\langle \delta O \right\rangle \) also makes it easy to choose a more elaborate windowing function should this be desired.

Figure 2. Contribution to \( \left\langle \delta O \right\rangle \) of correlator between \( \langle \delta S[U] \rangle_y = \langle n_f \log M[U] \rangle_{yy} \) and \( (W_{11})_x \) to \( \left\langle \delta O \right\rangle \)

6. Approximating full QCD by shifting the gauge coupling and expanding \( \langle \text{Tr} \log M \rangle \)

Following [5] and identifying
\[ \delta S = n_f \text{Tr} \log M - \delta \beta \text{S}_{\text{gauge}} \]  
(18)

we again look at corrections to Wilson loops. These are measured on a set of 200 \( 10^4 \) full QCD configurations with \( \beta = 5.679 \), \( \kappa = 0.16 \) and \( n_f = 2 \) and also the set of quenched QCD configurations used earlier. The results are shown
in Fig. 3 and are in accordance with [5]. A notable difference between the two is the computational savings afforded by the choice of algorithm for $\text{Tr} \log M$. Use of unbiased subtractors means that only 10 noise vectors are needed. In addition to this we do not have to fix the configurations to Landau gauge.

The previously mentioned method of cutting the integral off to reduce the statistical error turns out not to work for $\delta S$ defined in (18). The contributions from $\text{Tr} \log M$ and $\delta \beta S_{\text{gauge}}$ are nearly equal but are opposite in sign and so the total correction is small as is shown in Fig. 3.

Introducing a cutoff reduces the contributions from $\text{Tr} \log M$ and $\delta \beta S_{\text{gauge}}$ by different amounts which produces a large variation in the total correction. This is shown in Fig. 3.

We have also looked at corrections to two point functions but the noise is such that this method cannot be used as is to provide improved mass measurements.

Figure 3. Corrections to Wilson loops relative to the full QCD value comparing the effectiveness with and without the cut off scheme.

Figure 4. Relative corrections to Wilson loops by expanding to first order in $\delta S = n_f \text{Tr} \log M - \delta \beta S_{\text{gauge}}$ as per (18).

7. Conclusion

A method of improving estimates of observables measured on quenched QCD configurations was tested on some sets of small ($10^4$) configurations. Expanding to first order in $\delta S = n_f \text{Tr} \log M$ gave moderate improvement to estimators for Wilson loops. Analysis of the source of the statistical error hinted at problems that the method would have on larger lattices and with two point functions, and also suggested a technique for its partial alleviation. The technique does have the potential to address these problems but at the price of reducing the size of the correction.
Figure 5. Relative corrections to Wilson loops from each component of $\delta S$ both separately and in combination.

It was shown in [5] that combining the above method with an appropriate shift in the gauge coupling can provide more accurate corrections to Wilson loop values. We obtained the same results using a more economical method of calculating $\text{Tr} \log M$.

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