The PZ method for estimating determinant ratios, with applications

C. Thron, K. F. Liu, and S. J. Dong

aDepartment of Physics and Astronomy, University of Kentucky, Lexington, KY 40506, USA

We introduce a new method for estimating determinants or determinant ratios of large matrices, which combines the techniques of Padé approximation with rational functions and $Z_2$ noise estimation of traces of large matrices. The method requires simultaneously solving several matrix equations, which can be conveniently accomplished using the MR method. We include some preliminary results, and indicate potential applications to non-Hermitian matrices, and Hybrid Monte Carlo without pseudofermions.

1. Introduction

The current work was motivated by our search for an alternative implementation of the Hybrid Monte Carlo (HMC) algorithm in Lattice QCD which does not require the use of pseudofermions. Our proposed algorithm (which is described in more detail in [1]) requires the estimation of determinant ratios $\det M_1 / \det M_2$ where the matrices $M_1$ and $M_2$ satisfy the following conditions: $M_1$ and $M_2$ are huge ($N \times N$, where $N \sim 10^6$); the eigenvalues of $M_1$ and $M_2$ have positive real parts; $\log(\det M_i)$ are $O(N)$, but det $M_1 / \det M_2$ is $O(1)$; and the eigenvalues of $M_2$ are continuous perturbations of the eigenvalues of $M_1$.

In this paper we present a new method for estimating such determinant ratios, which takes advantage of Padé approximation and $Z_2$ noise vectors (hence the acronym 'PZ'). The potential application of related methods to estimating the density of states is also indicated.

2. Outline of the PZ Method

Our improved algorithm is based on the approximation of $\log \lambda$ with a rational function via the use of Padé approximants. The Padé approximation to $\log(z)$ of order $[J, J]$ at $z_0$ is a rational function $N(z)/D(z)$ where $\deg N(z) = \deg D(z) = J$, whose value and first $2J$ derivatives agree with $\log z$ at the specified point $z_0$. When the Padé approximation is expressed in partial fractions, we obtain

$$\log M \approx a_0 I + \sum_{j=1}^{J} a_j (M + b_j)^{-1},$$

which implies

$$\log \{ \det M_1 / \det M_2 \} = Tr [\log M_1 - \log M_2]$$

$$= \sum_{j=1}^{J} a_j \{ Tr(M_1 + b_j)^{-1} - Tr(M_2 + b_j)^{-1} \}. \quad (2)$$

The traces of inverse matrices $(M + b_j)^{-1}$ may then be found using the $Z_2$ noise method [3], and it follows

$$Tr [\log M_1 - \log M_2] \approx \frac{1}{L} \sum_{j,l} a_j \eta_l (\xi_{j,l}^{(1)} - \xi_{j,l}^{(2)}), \quad (3)$$

where $\{ \eta_l, l = 1, \ldots, L \}$ are complex $Z_2$ noise vectors, and the $\xi_{j,l}^{(k)}$ are vectors defined by:

$$\xi_{j,l}^{(k)} = (M_k + b_j I)^{-1} \eta_l. \quad (4)$$

3. Advantages of the PZ method

The PZ method takes advantage of proven, effective numerical approximation techniques. Padé approximation uses rational functions, which are very efficient when it comes to uniform approximation of analytic functions: for example, an $[11, 11]$ Padé expansion of $\log z$ around $z_0 = 0.1$ is accurate to within $10^{-7}$ on the interval $[0.04, 2.5]$. In our application, the Padé approximation to the logarithm only needs to be accurate on the region in the complex plane where the
spectra of $M_1$ and $M_2$ differ. Also, complex $Z_2$ random vectors have been shown to be superior to Gaussian in computing traces of inverse matrices.

The PZ method is also in a position to take advantage of recent results on efficient solution of linear problems with multiple diagonal shifts. The column inversions in (4) for fixed $l, k$ may be performed using GMRES with multiquarks in the same computational time it takes to solve just one–only more memory is required (an additional vector for each $j$) [3]. This can lead to a considerable speedup in the algorithm. Hence, a higher order Padé expansion requires more memory, but the same computation time (apart from matrix conditioning effects, see next paragraph). The multi-quark GMRES method can be applied to non-Hermitian matrices: so determinants of non-Hermitian matrices may also be found directly, without recourse to the Hermitian matrix $M^* M$.

The $b_j$’s turn out to have positive real parts, and negligible imaginary parts: thus the matrices $M + b_j I$ are better- conditioned than $M$, and the column inversions should be faster.

However, this effect diminishes for higher order Padé approximations, because the real parts of some terms become smaller.

The PZ method also holds promise of being useful in the case where different quark flavors are present, in which case it is necessary to compute

$$\frac{\det \{(M_1 + \mu_1)(M_1 + \mu_2)\}}{\det \{(M_2 + \mu_1)(M_2 + \mu_2)\}}$$

Using multi-quark GMRES, this takes the same amount of computation as a single determinant ratio.

4. Numerical Results

Figure 1 shows the result of numerical experiments involving the matrix $M_1$ associated with a typical (heatbath-generated) quenched gauge configuration on a $16^3 \times 24$ lattice with $\beta = 6.0$, $\kappa = 0.154$, and the matrix $M_2$ generated from $M_1$ by updating 20 links in a heatbath. The PZ estimates of $\log (\det M_1) / (\det M_2)$ using (1) with an additional term $a_0 N$ and $\xi_j^{(2)} = 0$ is shown in Figure 3, while the corresponding jackknife errors are shown in Figure 4. The PZ estimate of the imaginary part of $\log (\det M_1)$ is shown in Figure 5 (the actual value is 0).

These results demonstrate that the PZ method leads to controlled error in determinant ratios after a relatively small number of column inversions.

5. Numerical error and computation time in the PZ method

There are three sources of numerical error in the PZ method: Padé approximation; $Z_2$ estimation; and column inversion via GMRES. The Padè error can be virtually eliminated by taking more terms in the Padè expansion, which requires more memory but not more computation time. A theoretical expression for the $Z_2$ error is

$$\text{Var}(Tr A - Tr \eta^\dagger A \eta) = \frac{1}{L} \sum_{i \neq j} \|A_{ij}\|^2.$$  \hspace{1cm} (6)

The column inversion error is reduced by taking more iterations, at the cost of increased computation time.
3

The computation time depends on the number of noise vectors required to get a good trace estimate. If GMRES is used, each noise vector used gives rise to one column inversion.

It should be mentioned that alternatives to Padé approximation have been proposed, including Chebyshev polynomials \([5]\) and Stieltjes integrals \([6]\). Numerical experiments should be performed to determine which is more efficient.

6. Estimating the density of states

Some of the ideas introduced above may be used to estimate the density of states \(\rho(\lambda)\) as follows. Any term of the form

\[
Tr\{(M - b_j)^{-1}\} = \sum_{n=1}^{N} \frac{1}{\lambda_n - b_j} = \int \int d^2\lambda \frac{1}{\lambda - b_j} \rho(\lambda)
\]

(7)

can be used as a “probe” to sample spectral information near the specified pole \(b_j\). Hence \(\rho(\lambda)\) can be estimated via the following procedure: (1) Choose \(J\) complex numbers \(b_j\) which are strategically placed around the support of \(\rho(\lambda)\); (2) Estimate \(T_j \equiv Tr\{(M - b_j)^{-1}\}\) using the \(Z_2\) noise method; (3) Specify a fitting form for \(\rho(\lambda)\) using \(J\) parameters: \(\rho(\lambda) \approx \sum_{j=1}^{J} p_j \phi_j(\lambda)\); and (4) Find the parameters \(p_j\) by solving the equations

\[
T_j = \sum_{j=1}^{J} p_j \int [d^2\lambda] \frac{\phi_j(\lambda)}{\lambda - b_j}.
\]

(8)

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Figure 4. Jackknife error for estimates in Figure 3.

Figure 5. PZ estimate of imaginary part of $\log(\det M)$. 
