Approximate actions for dynamical fermions

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Recent developments and applications of approximate actions for full lattice QCD are described. We present first results based on the stochastic estimation of the fermion determinant on $12^3 \times 24$ configurations at $\beta = 5.2$.

1. BASIC PRINCIPLES

Consider actions $S_1[U]$ and $S_2[U]$ describing two lattice gauge theories with the same gauge configuration space $\{U\}$ so that ($i = 1, 2$)

\[ Z_i \equiv \int \mathcal{D}U e^{-S_i[U]}, \quad < F >_i \equiv \frac{1}{Z_i} \int \mathcal{D}U e^{-S_i} . \tag{1} \]

For example, $S_1$ might be the quenched Wilson action and $S_2$ the SW-improved action for 2-flavour QCD. Here, $F$ is some operator. Expectation values in the two theories can be related via a cumulant expansion whose leading behaviour implies $^[1]$

\[ < F >_2 = < F >_1 + < \tilde{F} \Delta_{12} > + \ldots \tag{2} \]

where $\Delta_{12} \equiv S_1 - S_2$, $\tilde{F} \equiv F - < F >$ etc. \(^\tag{3}\)

In general, an action is a function of several parameters, e.g. the Wilson action depends on the bare parameters $\beta$ and $\kappa$. One may consider matching different actions in one of several ways $^[1]$:

- **M1**: minimise the ‘distance’ between the actions, i.e. $\sigma^2(\Delta_{12})$;

- **M2**: match a given set of operators. i.e. require $< F_n >_1 = < F_n >_2$;

- **M3**: maximise the acceptance in an exact algorithm for $S_2$ constructed via accept/reject applied to configurations generated with action $S_1$.

It turns out that, to lowest order, these 3 tuning prescriptions coincide. They differ in a calculable way at next order. Details are in $^[1]$.

2. APPLICATIONS TO QCD

2.1. Tuning action parameters

In $^[1]$, we demonstrated how a relatively modest number of Wilson loop operators (three or four)

\[ S_1 = - \sum_{i=1}^n a_i \tilde{W}_i \tag{4} \]

can be used to approximate the full Wilson action $S_2 = S_G - T$ where $T \equiv \frac{nf}{2} \text{TrLn}[M^1 M]$ . \(^\tag{5}\)

A particularly simple application is to study the quenched approximation (see also $^[2]$). Here $n = 1$ and $W_1 \approx S_G$, the usual Wilson gauge action. Tuning the quenched coupling $\beta_Q$ in $S_1$ to match $S_2$ (full QCD) at a given $\beta$ and $\kappa$ yields (at first order):

\[ \delta \beta \equiv \beta - \beta_Q = - \frac{< \tilde{T} \tilde{W}_1 >}{< \tilde{W}_1^2 >} . \tag{6} \]

In general, one requires a better range of loop operators $^[1]$ or, indeed, other types of operators to capture the essential physics. In all cases, the basic principles and techniques are the same.
2.2. Bare parameter dependence in QCD

Another practical application is to take

\[ S_1 = S_{QCD}(\beta_0, \kappa_0) \quad \text{and} \quad S_2 = S_{QCD}(\beta, \kappa) \]  

so as to explore the bare parameter dependence of the lattice theory using configurations generated at a finite number of reference points \((\beta_0, \kappa_0)\) in parameter space. For example, at fixed \(\beta = \beta_0\), one might wish to explore the \(\kappa\)-dependence of measurements. According to eqn. \[3\] one requires measurements of

\[ \Delta_{12} = S_1 - S_2 = T(\kappa) - T(\kappa_0). \]  

One can make stochastic estimates of this quantity quite efficiently (see section \[3\]) - certainly much more rapidly than by performing independent dynamical fermion simulations at each set of parameters.

2.3. Exact algorithm for full QCD

In \[3\], we constructed an algorithm which delivers configurations correctly distributed with respect to a desired action \(S_2\) as follows:

\[ \mathcal{W}_2(U, U') \equiv \mathcal{W}_1(U, U') A(U', \Delta_{12}[U']). \]  

The acceptance probability \(A\) depends directly on the quality of the approximate action \[3\]:

\[ A(\Delta_{12}) = \text{erfc}(\frac{1}{2} \sqrt{\sigma^2(\Delta_{12})}). \]  

The action difference \(\Delta_{12}\) is of course an extensive quantity. In a typical application, the transition probability \(\mathcal{W}_1\) for the approximate action should correspond to a relatively fast update scheme. Application of this idea to full QCD may offer a partial solution to decorrelation problems with standard dynamical fermion algorithms.

3. STOCHASTIC ESTIMATES OF THE FERMION DETERMINANT

We require an unbiased estimator for \(\text{TrLn}H\) where \(H = M^T M\) is a hermitian positive-definite matrix. Bai, Fahey and Golub \[4\] have recently proposed estimators, with bounds, for quantities of the form

\[ u^T f(H)v \]  

where, for example in our case, \(f = \text{Ln}\). Taking \(u = v\) as some normalised noise vector (e.g. \(Z_2\)), we can obtain a stochastic estimate of \(\text{TrLn}H\).

The efficiency of the method, in comparison with the Chebychev-based methods used previously \[20\] results from an elegant relationship between the nodes/weights required for a \(N\)-point Gaussian quadrature and the eigenvalues/eigenvectors of a Lanczos matrix of dimension \(N\) \[3\]. This relationship and resulting accuracy appears to remain good, when orthogonality is lost in standard numerical Lanczos methods. In the present case, for a fixed noise vector we obtain 6 figure convergence of the quadrature with 70 Lanczos steps on a matrix with condition number of order \(10^4\). The estimator of \(T \equiv \text{TrLn}H\) is of the form

\[ E_T = \frac{1}{N^2} \sum_{i=1}^{N^2} I(\phi_i), \quad I(\phi_i) = \sum_{j=1}^{N} \omega_j \text{Ln}(\lambda_j) \]  

where \(\{\lambda_j\}\) are eigenvalues of the tridiagonal Lanczos matrix arising using \(\phi_i\) as a starting vector and \(\{\omega_j\}\) are related to the corresponding eigenvectors. Details of the method will be presented elsewhere \[4\].

4. QCD RESULTS AT \(\beta = 5.2\)

4.1. Quenched comparisons

In Table \[4\] we show the results of matching quenched and SW-improved \[4\] fermion actions using eqns. \[3\] \[3\]. The errors on comparison val-

| \(\kappa\) | Configs. | \(<P>\) | \(\beta Q\) | \(<P>_{Q}\) |
|---|---|---|---|---|
| .136 | 100 | .4874(1) | 5.48(2) | .488(4) |
| .139 | 40 | .5160(2) | 5.62(2) | .530(4) |

uses of \(<P>_{Q}\) include those associated with the uncertainty in estimating \(\beta Q\). The comparison at the heavier quark mass, \(\kappa = .136\), shows complete consistency \((\approx 0.488)\). That at the lighter
quark mass is close but not precise. It is seen from this and from other results that, at $\kappa = .139$, one may be starting to see non-trivial effects of unquenching.

4.2. Static potential measurements

To probe dynamical quark effects more closely, we have studied the static potential on quenched ($\beta_Q = 5.7$) and on 2 flavour dynamical fermions configurations ($\beta = 5.2$) at several values of $\kappa$. Measurements were made using the optimised techniques of [3]. Results for $V(R)$ and the extraction of the lattice spacing via $r_0$ [7] are presented elsewhere [8]. Strong scale dependence on $\kappa$ is observed. We used eqns. 3 and 8 (working to lowest order) to ‘predict’ the $\kappa = .139$ potential from that measured at $\kappa = .136$ where the quarks are effectively much heavier. There was evidence that the lowest order correction captures much of the change in behaviour but with large errors. This is not surprising since making comparisons at fixed $\beta$ involves different physical scales.

4.3. Estimating ‘distances’

In Table 2, we show the distance (squared) $\sigma^2(\Delta_{12})$, as defined in section 4, between our dynamical fermion reference action at $\beta_0 = 5.2$, $\kappa_0 = .136$ and other relevant actions. For example, the second line shows the quality of the quenched tuning described above (see Table 1): a reduction from 9250 to 855 by shifting $\beta$. Also, we note that $\kappa = .139$ is some distance (147) from the reference $\kappa_0 = .136$. This is the origin of the difficulty (noted above) in predicting $\kappa = .139$ results from .136 configurations without also tuning $\beta$. The last line of the table shows that operator matching should be much closer using ($\beta_0, \kappa_0) = (5.2, 0.136)$ and ($\beta, \kappa) = (5.165, 0.139)$, since the estimated distance is only $17 \pm 3$. This could be checked directly with further simulations at $\beta = 5.165, \kappa = .139$. We would expect the lattice spacing to be similar at these two points in action parameter space.

4.4. Approximate loops actions

We have begun a systematic study of possible approximate actions constructed from Wilson loops. Initially, we have chosen to construct these from a range of link steps of size 1, 2, 3, 4 etc. The aim is to minimise the distance between the target action, e.g. full QCD at $\beta_0 = 5.2$ and $\kappa_0 = .136$ in the present example, and the parametrised loop action [4]. It is not hard to reduce the distance well below that achieved with a single plaquette (see Table 2). However, eqn. 10 shows, for example, that $\sigma^2$ must be less than 10 to give an acceptance greater than 2.5%, in the corresponding exact algorithm.

Further work will include: continuing studies to establish more efficient loop operators and other classes of approximate action; studies of the parameter space of standard dynamical fermion actions; mapping the parameter spaces of different types of action.

Table 2

| Action | $\beta$ | $\kappa$ | ‘Distance’ |
|--------|---------|----------|------------|
| Quen.  | 5.2     | –        | 9250(1330) |
| Quen.  | 5.479(15)| –        | 855(255)   |
| $N_f = 2$ | 5.2     | .139     | 147(20)    |
| $N_f = 2$ | 5.165(1)| .139     | 17(3)      |

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