Lanczos Methods for UV-Suppressed Fermions
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In this talk I introduce lattice fermions with suppressed cutoff modes. Then I present Lanczos based methods for stochastic evaluation of the fermion determinant.

1. INTRODUCTION

There has been recent interest in the so-called ‘Ultraviolet slowing down’ of fermionic simulations in lattice QCD [1–5]. These studies try to address algorithmically large fluctuations of the high end modes of the fermion determinant. The goal is to increase the signal-to-noise ratio of the infrared modes and to accelerate fermion simulations as well.

In fact, all the computational effort needed to treat UV-modes by above algorithms can be reduced to zero by suppressing them in the first place [6]. The lattice Dirac operator of this fermion theory is given by:

\[ D = \mu a \Gamma_5 \tanh \frac{a \Gamma_5 D_{W/s/o}}{\mu} \]  

where \( D_{W/s/o} \) is the input lattice Dirac operator, \( a \) the lattice spacing and \( \mu > 0 \) is a dimensionless parameter. For Wilson (W) and overlap (o) fermions as the input theory one has \( \Gamma_5 = \gamma_5 \). For staggered fermions \( \Gamma_5 \) is a diagonal matrix with entries \(+1/−1\) on even/odd lattice sites. The theory converges to the input theory in the continuum limit and is local and unitary as shown in detail in [6]. The input theory is also recovered in the limit \( \mu \to \infty \). For \( \mu \to 0 \) one has \( D \to \mu \), i.e. a quenched theory.

Perturbative calculations with this theory are straightforward. In the following Wilson fermions are used as input. The inverse fermion propagator is given by:

\[ \tilde{D}(p) = \frac{\mu}{a \gamma_5} \tanh \frac{a \tilde{H}_W(p)}{\mu} \]  

with \( p = \{ p_\nu, \nu = 1, \ldots, 4 \} \) being the four-momentum vector. As usual, gauge fields are parametrized by \( su(3) \) elements, \( U(x)_\nu = e^{i a g A(x)_\nu} \) with \( A(x)_\nu \in su(3) \) algebra, and the Wilson operator is written as a sum of the free and interaction terms: \( D_W = D_W^0 + D_W^I \). The splitting of the lattice Dirac operator is written in the same form:

\[ D = D^0 + D^I, \quad D^0 = \frac{\mu}{a \gamma_5} \tanh \frac{a H_W^0}{\mu} \]  

where the interaction term has to be determined. This can be done by expanding \( D \) in terms of \( a/\mu \):

\[ D = D_{W} \left[ 1 + c_1 \left( \frac{a H_W}{\mu} \right)^2 + c_2 \left( \frac{a H_W}{\mu} \right)^4 + \ldots \right] \]  

where \( c_1, c_2, \ldots \) are real expansion coefficients. Calculation of \( D^I \) is an easy task if one stays with a finite number of terms in the right hand side of (3). Also, the number of terms can be minimized using a Chebyshev approximation for the hyperbolic tangent. \(^1\)

2. COMPUTATIONAL METHODS

The effective action of the theory defined above can be written as:

\[ S_{\text{eff}} = \text{tr} f(A) \]  

where \( A \in \mathbb{C}^{N \times N} \) and \( f(s) \) is a real and smooth function of \( s \in \mathbb{R}^+ \). The matrix \( A \) is assumed

\(^1\)I would like to thank Joachim Hein for discussions related to lattice perturbation theory.
to be Hermitian and positive definite. Since the trace is difficult to obtain one can use the stochastic method of [7]. The method is based on evaluations of many bilinear forms of the type:

$$\mathcal{F}(b, A) = b^T f(A)b$$  \hspace{1cm} (5)

where $b \in \mathbb{R}^N$ is a random vector. The trace is estimated as an average over many bilinear forms. A confidence interval can be computed as described in detail in [7]. Here I will describe an alternative derivation of the Lanczos algorithm [8], which is used in [7] and in [9] as well. The full details of this study can be found at [10]. It is easy to see that the QL method delivers the extreme eigenvalues of the original matrix $A$. In the application considered here one can show that [10]:

$$\sum_{k=1}^{m} b^T \frac{c_k}{A + d_k \mathbb{I}} b = ||b||^2 \sum_{k=1}^{m} \frac{c_k}{T_n + d_k \mathbb{I}} e_1$$  \hspace{1cm} (8)

where $\mathbb{I}_n \in \mathbb{R}^{n \times n}$ is the identity matrix and $e_1$ is its first column. From this result and the convergence of the partial fractions to the matrix function $f(\cdot)$, it is clear that:

$$\mathcal{F}(b, A) \approx \tilde{\mathcal{F}}_n(b, A) = ||b||^2 c^T f(T_n)e_1$$  \hspace{1cm} (9)

Note that the evaluation of the right hand side is a much easier task than the evaluation of the right hand side of (5). A straightforward method is the spectral decomposition of the symmetric and tridiagonal matrix $T_n = Z_n \Omega_n Z_n^T$, where $\Omega_n \in \mathbb{R}^{n \times n}$ is a diagonal matrix of eigenvalues $\omega_1, \ldots, \omega_n$ of $T_n$ and $Z_n \in \mathbb{R}^{n \times n}$ is the corresponding matrix of eigenvectors, i.e. $Z_n = [z_1, \ldots, z_n]$. From (9) and the spectral form $T_n = Z_n \Omega_n Z_n^T$ it is easy to show that:

$$\tilde{\mathcal{F}}_n(b, A) = ||b||^2 c^T Z_n f(\Omega_n) Z_n^T e_1$$  \hspace{1cm} (10)

where the function $f(\cdot)$ is now evaluated at individual eigenvalues of the tridiagonal matrix $T_n$. The eigenvalues and eigenvectors of a symmetric and tridiagonal matrix can be computed by the QL method with implicit shifts [12]. The method has an $O(n^3)$ complexity. Fortunately, one can compute (10) with only an $O(n^2)$ complexity. Closer inspection of eq. (10) shows that besides the eigenvalues, only the first elements of the eigenvectors are needed:

$$\tilde{\mathcal{F}}_n(b, A) = ||b||^2 \sum_{i=1}^{n} z^T_i f(\omega_i)$$  \hspace{1cm} (11)

It is easy to see that the QL method delivers the eigenvalues and first elements of the eigenvectors with $O(n^2)$ complexity. A similar formula (11) is suggested by [7] based on quadrature rules and Lanczos polynomials. Clearly, the Lanczos algorithm is implemented in [12].

I thank Alan Irving for the related comment on the QL implementation in [12].
Algorithm 1: Lanczos algorithm to compute (5).

Set $\beta_0 = 0$, $\rho_1 = 1/||b||_2$, $q_0 = o$, $q_1 = \rho_1 b$

for $i = 1, \ldots$ do

$v = Aq_i$

$\alpha_i = q_i^\dagger v$

$v := v - \alpha_i q_i - q_{i-1} \beta_{i-1}$

$\beta_i = ||v||_2$

$q_{i+1} = v/\beta_i$

$\rho_{i+1} = -(\rho_i \alpha_i + \rho_{i-1} \beta_{i-1})/\beta_i$

if $1/|\rho_{i+1}| < \epsilon$ then

$n = i$

stop

end if

end for

Set $(T_n)_{i,i} = \alpha_i$, $(T_n)_{i,i+1} = \beta_i$

otherwise $(T_n)_{i,j} = 0$

Compute $\omega_i$ and $z_{1i}$ by the QL method

Evaluate (5) using (11)


diagram text

Figure 1. Relative differences of (11) (solid line), the largest (dashed line) and the smallest eigenvalue (dotted line) of $T_n$ for $f(s) = \log(\tanh(\sqrt{s}))$, $s > 0$, $A = H_W^2$, and $b \in \mathbb{Z}_2$. noise on a $12^4 \times 24$ lattice at $\beta = 5.9$ and bare Wilson quark mass $m = -0.869$.

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