Minimizing storage in implementations of the overlap lattice-Dirac operator.

Herbert Neuberger
neuberg@physics.rutgers.edu

Department of Physics and Astronomy
Rutgers University
Piscataway, NJ 08855–0849

Abstract

The overlap lattice-Dirac operator contains the sign function $\epsilon(H)$. Recent practical implementations replace $\epsilon(H)$ by a ratio of polynomials, $H P_n(H^2)/Q_n(H^2)$, and require storage of $2n + 2$ large vectors. Here I show that one can use only 4 large vectors at the cost of executing the core conjugate algorithm twice. The slow-down might be less than by a factor of 2, depending on the architecture of the computer one uses.
The overlap [1, 2] has produced a new lattice Dirac operator [3, 4]. Using this operator one can define QCD on the lattice with explicit exact global chiral symmetries. Full, exact chiral symmetry on the lattice without fine tuning could not be achieved with previous lattice Dirac operators. The new operator is given by:
\[ D = \frac{1 + \gamma_5 \epsilon(H)}{2}, \]  
(1)
where \( H = \gamma_5 D' \). There is some freedom in choosing \( D' \). The simplest choice is \( D' = D_W \). \( D_W \), the Wilson-Dirac operator, in \( d \geq 3 \)-dimensions, is taken with hopping parameter \( \kappa \) close to the middle of the allowed range \( \left( \frac{1}{2d}, \frac{1}{2d-4} \right) \). Choosing \( D' = D_W \) maximizes the sparseness of \( H \) and thus minimizes the cost of evaluating \( Hb \) for generic vectors \( b \).

Recent implementations of the overlap lattice Dirac operator [5, 6] employ a sum of terms of the form \( \frac{1}{H^{s+\sigma^s}} \) with \( s = 1, \ldots, n \) and \( 0 < \sigma^1 < \sigma^2 \ldots < \sigma^n \):
\[ \epsilon(H) = \lim_{n \to \infty} \frac{H}{n} \sum_{s=1}^{n} w^s \frac{1}{H^2 + \sigma^s}. \]  
(2)
Using the method of multiple shifts [7], the number of \( H^2p \) operations required to evaluate the action of the right hand side of equation (2) on vectors \( p \) for arbitrary finite \( n \) becomes independent of \( n \). Actually, the number of operations is not much more than required to compute \( \frac{1}{H^{s+\sigma^s}}b \) by the simple conjugate gradient (CG) algorithm [8]. This saving comes at some expense: one needs to store \( 2n + 2 \) vectors.

The main objective of this paper is to suggest a way to avoid storing \( 2n + 2 \) vectors. For large lattices this might be necessary. The saving in storage comes at the price of executing two passes over the basic CG algorithm instead of a single pass. Thus, at the cost of doubling the amount of \( H^2p \) operations, storage also becomes almost \( n \) independent, and does not exceed substantially the requirements of computing \( \frac{1}{H^{s+\sigma^s}}b \) by CG. The basic trick is similar to the way large storage demands are avoided if one uses the Lanczos method [9] to compute not only eigenvalues but also a few eigenvectors.

Below, I shall first review the single-pass method following the notations and methods of Jegerlehner [7]. Next, I construct the two-pass method. I end discussing possible advantages of using the two-pass implementation.

For large enough \( n \), typically, \( \sigma^1 \) is so small relative to the lowest eigenvalue of \( H^2 \) that nothing is lost by driving the algorithm with the inversion of \( H^2 \) itself, rather than \( H^2 + \sigma^1 \). In any case, the algorithm is easily altered to make \( H^2 + \sigma^1 \) the driver. Below, I use just \( H^2 \). I assume that a vector \( b \) is given and my objective is to compute \( \epsilon(H)b \).

**Pseudocode for the single-pass version.**
Vector variables: \( r, p, x^s, p^s \).
Scalar variables: \( \alpha, \beta, \zeta^s, \rho, \) tolerance, \( b_{\text{norm}} \).

Initialize: \( r_0 = b, p_0 = b, \) \( b_0 = (b,b) \), \( b_{\text{norm}} = \sqrt{\rho_0} \), \( \alpha_0 = 0, \beta_{-1} = 1 \), for \( s = 1,2,..,n \) \( \{ x_0^s = 0, p_0^s = b, \, \zeta_{-1}^s = 1, \, \zeta_0^s = 1 \} \).

Iterate: for \( i = 0,1,2,3,..: \)

\[
\{ \\
\text{i. for } s = 1,2,...n: \\
\quad \begin{aligned} \\
& w_i = H^2 p_i \\
& \beta_i = -\rho_i/(p_i, w_i) \\
& \zeta_{i+1} = \frac{\zeta_{i} \zeta_{i-1} \beta_{i-1}}{\beta_{i} \alpha_i (\zeta_{i-1} - \zeta_{i}) + \zeta_{i-1} \beta_{i-1} (1 - \beta_{i} \sigma^s)} \\
& x_{i+1}^s = x_i^s - \beta_i (\zeta_{i+1}/\zeta_i^s)p_i^s \\
\end{aligned} \tag{A} \\
\} \\
\quad r_{i+1} = r_i + \beta_i w_i \\
\quad \rho_{i+1} = (r_{i+1}, r_{i+1}) \\
\quad \alpha_{i+1} = \rho_{i+1}/\rho_i \\
\quad p_{i+1} = r_{i+1} + \alpha_{i+1} p_i \\
\} \\
\text{ii. for } s = 1,2,...n: \\
\{ \\
\quad p_{i+1}^s = \zeta_{i+1}^s r_{i+1} + \alpha_{i+1} (\zeta_{i+1}^s/\zeta_i^s)^2 p_i^s \tag{B} \\
\} \\
\text{If } \sqrt{\rho_{i+1}} < \text{tolerance} \cdot b_{\text{norm}}, \text{ exit.} \\
\}

Let me make a few comments on the algorithm:

- The denominator in line (A) above will underflow for larger \( \sigma^s \) before convergence has been reached for the lower \( \sigma^s \). In practice the number of already converged \( s \)-values is stored and updated, so for any \( s \) the CG algorithm is not executed past convergence.
- Line (B) differs slightly from the explicit pseudo-code in [7].
- If one uses \( H^2 + \sigma^1 \) as driver in \( H^2 \)’s stead, \( p \) can be replaced by \( p^1 \), resulting in some small saving.
- The core conjugate gradient constitutes of what is left of the above after the blocks i and ii are excluded.
We are only interested in obtaining a numerical approximation to the vector \( y = \epsilon(H)b \): The output we need is the linear combination

\[
y_{i+1} = \sum_{s=1}^{n} w^s x^s_{i+1}.
\]  

In equation (3) I assumed that convergence of the CG procedure is achieved at step \( i + 1 \) for all \( s \). To avoid underflows, one sometimes needs to replace \( i \) by \( i_s \) where \( i_s \) is the \( s \)-dependent point of convergence. I sketched above how this is done.

It is obvious that we are not interested in the individual vectors \( x^s_{i+1} \), but only in one particular linear combination. The idea is then to calculate only the needed linear combination iteratively, without extra storage. Just as in the Lanczos case, this requires an extra pass over the core CG procedure.

Each \( x^s_{i+1} \) in equation (3) is a linear combination of the \( s \)-independent Krylov vectors \( r_j \). Thus, \( y_{i+1} \), which is all we care to know, is also a linear combination of \( r_j \)'s, and the single place \( s \)-dependence enters is in their coefficients. One cannot compute only the linear combination of equation (3) in one pass: The contributions from Krylov vectors computed in the early stages of the iteration enter with coefficients that are determined only in later iterations. Thus, a first pass is needed for the sole purpose of computing the coefficients \( \alpha_j \) and \( \beta_j \) up to the point where the driving CG process has converged. With this information, one can calculate the coefficients \( \zeta^s_j \) and also the points of convergence for the different masses (\( s \)-values). This information is used to compute all needed coefficients of the \( s \)-independent vectors \( r_j \) in the decomposition of \( y_{i+1} \).

The basic recursion determining the \( x^s_j \) can be read off the algorithm listed above:

\[
\begin{pmatrix}
  x^s_{j+1} \\
  p^s_{j+1}
\end{pmatrix} =
\begin{pmatrix}
  1 & -\beta^s_j \\
  0 & \alpha^s_{j+1}
\end{pmatrix}
\begin{pmatrix}
  x^s_j \\
  p^s_j
\end{pmatrix} + \zeta^s_{j+1} \begin{pmatrix}
  0 \\
  r^s_{j+1}
\end{pmatrix}.
\]  

In equation (4) \( \beta^s_j = \beta_j \zeta^s_{j+1}/\zeta^s_j \) and \( \alpha^s_{j+1} = \alpha^s_{j+1}(\zeta^s_{j+1}/\zeta^s_j)^2 \). Starting from equation (4) I derived the following expression:

\[
y_{i+1} = \sum_{k=0}^{i+1} R_k r_k
\]

\[
R_k = -\sum_{l=0}^{i-k} \beta_{k+l} \left( \prod_{j=1}^{l} \alpha_{k+j} \right) \sum_{s=1}^{n} \frac{\zeta^s_{k+l+1} \zeta^s_{k+l}}{\zeta^s_s}.
\]  

In equation (5) I adopted the convention that \( \prod_{j=1}^{0} \alpha_{k+j} \equiv 1 \). Again, the upper bounds on the sums over \( s \) in equation (5) must be altered to prevent underflows, but the information is available. So, in practice the sums over \( s \) only include the \( s \)-values that correspond to CG processes that have not yet converged at iteration \( k \).
Equation (5) clarifies why a single pass would not work without the extra storage: $R_k$, for low $k$’s, depends on $\alpha_j$, $\beta_j$, with $j$-values up to $i$. However, the coefficients $R_k, k = 0, ..., i + 1$ can be computed after the first pass. To compute $y_{i+1}$ we need the vectors $r_k$ and hence a second pass. In the second pass no inner products are required, since the coefficients $\alpha_j$ and $\beta_j$ are already known.

**Pseudocode for the two-pass version.**

Vector variables: $r, p, x$.
Scalar variables and arrays: $\alpha_j, \beta_j, \zeta^s_j, \rho, R_k$, tolerance, $b_{\text{norm}}$.

1. **First pass.**

   *Initialize:* $r_0 = b$, $p_0 = b$, $\rho_0 = (b, b)$, $b_{\text{norm}} = \sqrt{\rho_0}$, $\alpha_0 = 0$.

   *Iterate:* for $i = 0, 1, 2, 3, ...$:
   
   \[
   \begin{align*}
   w_i &= H^2p_i \\
   \beta_i &= -\rho_i/(p_i, w_i) \\
   r_{i+1} &= r_i + \beta_i w_i \\
   \rho_{i+1} &= (r_{i+1}, r_{i+1}) \\
   \alpha_{i+1} &= \rho_{i+1}/\rho_i \\
   p_{i+1} &= r_{i+1} + \alpha_{i+1} p_i
   \end{align*}
   \]

   If $\sqrt{\rho_{i+1}} < \text{tolerance } b_{\text{norm}}$, exit.

2. **Compute** $\zeta^s_j$ from line (A) in the single pass version, and $R_k$ from equation (5).

3. **Second pass.**

   *Initialize:* $r_0 = b$, $p_0 = b$, $x_0 = R_0 b$.

   *Iterate:* for $k = 0, 1, 2, 3, ... i$:
   
   \[
   \begin{align*}
   w_k &= H^2p_k \\
   r_{k+1} &= r_k + \beta_k w_k \\
   p_{k+1} &= r_{k+1} + \alpha_{k+1} p_k \\
   x_{k+1} &= x_k + R_{k+1} r_{k+1}
   \end{align*}
   \]
For large enough lattices one might expect the second version to take twice as long as the first. However, the nonuniform architecture of the memory is crucial and the actual efficiency attainable in practice can vary. I used a high level Fortran 90 code modeled on a package described in [10] and ran it at 64 bit precision on an SGI O2000 with four processors, each with 4MB cache memory. All parallelizations were done using automatic options. I tested the methods on a three dimensional system with gauge group $SU(2)$, two flavors [5], and lattice size $8^3$. I used gauge configurations generated from the single plaquette gauge action with coupling $\beta = 3.5$ and evaluated several of the lowest eigenvalues of $DD^\dagger$. $n$ was set to 32. This computation is of the same order of magnitude as a few $D$-inversions. I found that the second method actually ran faster by 30% than the first, at the same accuracy. The observed speed-up instead of the expected slow-down most likely reflects cache usage. Carefully optimized codes ought to show at least some slow-down in the two-pass method. This slow-down will not exceed a factor of 2.

The above test was done using the original method of [5], rather than the refined version of [6]. In the original method, the quantities $w_s$ and $\sigma_s$ are extracted from [11]:

$$\epsilon(H) = \lim_{n \to \infty} \frac{H}{n} \sum_{s=1}^{n} \frac{1}{H^2 \cos^2 \frac{\pi}{2n} \left(s - \frac{1}{2}\right) + \sin^2 \frac{\pi}{2n} \left(s - \frac{1}{2}\right)}.$$  \hspace{2cm} (6)

In the refined version of [6] different weights $w^*_s$ and pole locations $-\sigma^*_s$ are used. The advantage of the refinement is claimed to be that similar accuracies can be achieved with smaller values of $n$. This does not come entirely for free though. In the original method the spectrum of $\epsilon(H)$ is approached from within the interval $(-1, 1)$ while in the refined method of [6] the approach is oscillatory around $\pm 1$. Even tiny excursions of the spectrum of $\gamma_5 \epsilon(H)$ below $-1$ can cause problems when one inverts $D$. In the two-pass method the dependence of the overall computational cost on $n$ has been sufficiently weakened to make the original version of the rational approximation possibly more attractive.

In a recent paper [12] another method was presented, also requiring no extra storage. This new method employs a Lanczos iteration (similar to CG) to tridiagonalize $H$. Next, the square root of the relatively small triangular matrix is taken by some spectral method (this is similar to old implementations of the overlap [13]). To compute the action of the approximate $\epsilon(H)$ on a vector $b$ a second pass over the Lanczos procedure is needed. So, the ideas of using two passes in order to avoid extra storage are similar.

It is premature at the moment to decide which method is best; the answer may end up dependent on the particular architecture of the computer one uses. Therefore, it is useful to keep all possibilities in mind, and avoid getting locked into one particular implementation. New tricks producing large savings are still quite possible, given the limited time people
have been experimenting with implementations of $D$. In spite of the quite short time that has passed since [3], looking back to the first implementations in [13], followed by [14] where the Newton iteration was first applied, to more recent work [5, 6, 12], I find the amount of progress quite impressive.

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References.