Block Algorithms for Quark Propagator Calculation

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Computing quark propagators in lattice QCD is equivalent to solving large, sparse linear systems with multiple right-hand sides. Block algorithms attempt to accelerate the convergence of iterative Krylov-subspace methods by solving the multiple systems simultaneously. This paper compares a block generalisation of the quasi-minimal residual method (QMR), Block Conjugate Gradient on the normal equation, Block Lanczos and (\(\gamma_5\)-symmetric) Block BiConjugate Gradient.

1. Introduction

The calculation of quark propagators remains a major bottleneck in lattice QCD. The problem is to solve the matrix equation

\[ M\psi = \eta \]  

for \( \psi \) given several right-hand sides (sources) \( \eta \). The fermion matrix \( M \) is non-hermitian (we use Wilson fermions with clover improvement), sparse and very large. Recent attempts to accelerate the solution of Eq. (1) have focused on:

1. improved iterative methods
2. improved preconditioners, or
3. solving related systems.

There is growing consensus that the first of these areas is now mature \cite{1,2}, with BiCGSTAB emerging as the method to beat.

Finding a better preconditioner is complicated by the now universal requirement of scalability on parallel computers; red-black preconditioning (used in the present study) is beginning to give way to LL-SSOR \cite{3}, but the last word on preconditioning has not been said.

The third area is the exploitation of information found in the solution of one system to accelerate the convergence of another. Keeping the source fixed and varying \( \kappa \) leads to a family of multiple mass tricks \cite{4-6}. Keeping the matrix fixed and varying the source leads to the ideas of deflation \cite{1} and block algorithms, the several systems being solved simultaneously in the former but sequentially in the latter.

Two properties of \( M \) are relevant here.

1. \( M = \gamma_5 M^\dagger \gamma_5 \) is \( \gamma_5 \)-symmetric. This has been exploited to halve the computational costs of QMR and BiCG \cite{4}.
2. \( \frac{1}{\kappa} M \) is a shifted matrix with respect to its dependence on \( \frac{1}{\kappa} \). Multiple-mass tricks depend on this property.

Red-black preconditioning preserves property (1), but destroys property (2) except in the unimproved case of \( C_{SW} = 0 \).

2. Block Algorithms

Using a Krylov subspace method \( s \) times to solve \( s \) systems \( M\psi^{(1)} = \eta^{(1)}, \ldots, M\psi^{(s)} = \eta^{(s)} \) leads to the construction of several overlapping Krylov subspaces. In the worst case, i.e. when the number of iterations required for convergence equals the order \( N \) of \( M \), the overlap will be complete. By solving the \( s \) systems simultaneously, block algorithms eliminate the redundant matrix-vector operations in the above approach. One assembles the \( s \) right-hand sides into an \( N \times s \) matrix \( H = (\eta^{(1)}, \ldots, \eta^{(s)}) \) and solves

\[ M\Psi = H \]  

for \( \Psi = (\psi^{(1)}, \ldots, \psi^{(s)}) \).

On the other hand, a perfect preconditioner (one which coincides exactly with \( M^{-1} \)), solves the system with a single multiplication; in this case there is no gain to be had from the block algorithm. In practice we hope to have good preconditioners, so that we usually solve the point \( (s = 1) \) problem to the desired accuracy in much less than \( N \) multiplications. These considerations lead one
to expect that blocking will be most effective on badly conditioned systems and/or small volumes, i.e. when the number of iterations required for the point algorithm to converge is comparable to $N$. Blocking introduces certain overheads. The first is memory; the storage requirements for vectors in the point algorithm are multiplied by $s$ when going to the block algorithm. Secondly, vector-vector operations such as $y = αx + y$ and $β = y^Tx$ in the point algorithm generalise to $Y = Xα + Y$ and $β = Y^TX$ where $X$ and $Y$ are $N \times s$ matrices and $α$ and $β$ have become $s \times s$ matrices. The number of vector-vector operations required per iteration scales as $s^2$.

2.1. B-CGNNR and B-Lanczos

Block Conjugate Gradient [7] can be applied to the normal equation $M^TMΨ = M^TH$. Increasing $s$ yields a clear improvement in convergence, but not enough to defray the cost of squaring the condition number. Reference [8] studied a method based on the hermitian block Lanczos process and applied it to $γ_5 MΨ = γ_5 H$. B-Lanczos clearly outperforms B-CGNR. Unfortunately, $γ_5$ is a bad preconditioner for Eq. (2).

2.2. Block B-BiCG($γ_5$)

The algorithm presented here is a special case of, and easily derived from, the Block Bi-Conjugate Gradient algorithm of O’Leary [7]. I have used $γ_5$-symmetry to eliminate multiplications by $M^T$, and have followed her important suggestion of orthonormalising the columns of $P_k$.

**B-BiCG($γ_5$)**

\[
\begin{align*}
R_0 &= H - MΨ_0 \\
ρ_0 &= R^T_0 γ_5 R_0 \\
P_0 δ_0 &= R_0 \\
\end{align*}
\]

for $k = 0, 1, 2, \ldots$ until convergence do \{ \[
\begin{align*}
T &= MP_k \\
α_k &= \left( P^T_k γ_5 T \right)^{-1} δ^T_k ρ_k \\
Ψ_{k+1} &= P_k α_k + Ψ_k \\
R_{k+1} &= -T α_k + R_k \\
ρ_{k+1} &= P^T_{k+1} γ_5 R_{k+1} \\
β_k &= δ_k ρ_k ρ_{k+1} \\
T &= R_{k+1} + P_k β_k \\
P_{k+1} δ_{k+1} &= T
\end{align*}
\}

for $k = 1, 2, \ldots$ until convergence do \{ \[
\begin{align*}
δ_k &= V_k^T γ_5 V_k \\
β_k &= δ_k^{-1} ρ_k δ_k \\
T &= M V_k - V_k β_k \\
α_k &= δ_k^{-1} V_k^T γ_5 T \\
V_{k+1} &= T - V_k α_k \\
V_{k+1} ρ_{k+1} &= V_{k+1} δ_k \\
θ_k &= b_k - 2 β_k \\
e_k &= α_k - 1 d_k - 2 β_k + b_k - 1 α_k \\
ξ_k &= c_k - 1 d_k - 2 β_k + d_k - 1 α_k \\
\left( \begin{array}{c} α_k \\ β_k \\ Ψ_{k+1} \end{array} \right) &= \left( \begin{array}{c} c_k \\ d_k \\ 0 \end{array} \right) ξ_k \\
\left( \begin{array}{c} α_k \\ β_k \\ Ψ_{k+1} \end{array} \right) &= \left( \begin{array}{c} c_k \\ d_k \\ 0 \end{array} \right) ξ_k \\
V_k &= (V_k - P_{k-1} e_k - P_{k-2} θ_k)ξ_k^{-1} \\
τ_k &= a_k ξ_k, \quad ξ_k+1 = c_k ξ_k \\
Ψ_k &= Ψ_{k+1} + P_k τ_k \\
\end{align*}
\} \]

The operations (5) and (6) are QR decompositions, as are (7), (8) and (9) below.

2.3. Block QMR

The algorithm does not give a recurrence for the residual $R_k$, but the fact that $\text{Tr} \tilde{\tau}_k \tilde{\tau}_k$ is of the same order of magnitude as $\text{Tr} R_k^\dagger R_k$ is useful in formulating a stopping criterion.

This version does nothing to address the problems of Lanczos breakdown and (near) linear dependence in the columns of $V_k$. These can be brought under control, as shown in [11].

**3. Conclusions**

Block algorithms can reduce the number of matrix-vector operations required for convergence at the expense of more vector-vector operations. This does not necessarily lead to a reduction in wall-clock time.

B-QMR($\gamma_5$) and B-BiCG($\gamma_5$) are clearly faster than B-CGNR and B-Lanczos, and in some regimes (light masses and small volumes) they significantly outperform BiCGSTAB.

However, on lattices of realistic size, the improvements from blocking are marginal at best. At $\beta = 6.0$ quenched, $V = 16^3 \times 48$, I found that $s = 1$ is near-optimal for both B-QMR($\gamma_5$) and B-BiCG($\gamma_5$), unless the configuration is exceptional. At $\beta = 5.2$, $N_f = 2$, $V = 12^3 \times 24$, I found $s = 1$ to be optimal for the same algorithms at all $\kappa_{\text{valence}}$ and $\kappa_{\text{sea}}$ combinations studied in [12]. These conclusions should be reviewed if the relative cost of matrix-vector to vector-vector operations increases significantly. Block algorithms may yet have a role to play in conjunction with highly-improved actions on coarse lattices.

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