

Deflation of Eigenvalues for Iterative Methods in Lattice QCD

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Work on generalizing the deflated, restarted GMRES algorithm, useful in lattice studies using stochastic noise methods, is reported. We first show how the multi-mass extension of deflated GMRES can be implemented. We then give a deflated GMRES method that can be used on multiple right-hand sides of $Ax = b$ in an efficient manner. We also discuss and give numerical results on the possibility of combining deflated GMRES for the first right hand side with a deflated BiCGStab algorithm for the subsequent right hand sides.

1. INTRODUCTION

Removal of the smallest eigenvalues of a matrix can significantly improve the performance of iterative methods. This is important for lattice QCD where stochastic methods for disconnected diagrams and new matter formulations such as overlap fermions are computationally intensive. In addition, there is often a need for these systems to be shifted to take account of multiple quark masses or other parameters. We think that it is important for any iterative method we develop to be applicable to general non-Hermitian systems, for this is often the case for lattice systems.

GMRES [1] is an iterative method that can be used in lattice studies with stochastic noise methods. Convergence can be improved by deflating eigenvalues. Two years ago it was shown that deflating eigenvalues [2] can be especially helpful for lattice problems with multiple right-hand sides [3]. Here we report on generalizations of these techniques. First we show how deflated restarted GMRES can accommodate multiple shifts. We give numerical results for a Wilson matrix with very small eigenvalues. We then consider the case of combining multiple shifts with multiple right-hand sides. Finally we also discuss and give numerical results on the possibility of combining deflated GMRES for the first system with a BiCGStab algorithm which uses those deflated eigenvalues for the subsequent solutions.

2. DEFLATION FOR MULTIPLY SHIFTED SYSTEMS

The shifted systems are expressed by

$$(A - s(i)I)x^i = b, \quad (1)$$

where the $s(i)$ are the numerical shifts. The method proposed in [4] is based upon keeping the residual vectors for the shifted systems parallel to one another. That is, one uses only a single Krylov subspace to solve all the systems. This is possible for GMRES only by forcing the residuals to be parallel to one another after a restart and thus the minimum residual condition is applied to only the unshifted (most difficult) system. We find that this also results in an almost optimal solution for the shifted systems.

Our method for deflating GMRES (called GMRES-DR [3]) simultaneously solves linear equations and computes eigenvalues. This is possible because it has a Krylov subspace for solving the linear equations as well as Krylov subspaces designed for solving the eigenvalue equation. These approximate eigenvectors are refined and improved as the GMRES-DR cycles proceed. We have determined that GMRES-DR can be efficiently applied to multiply shifted systems because of its Krylov properties.

Fig.1 shows the result of a shifted run of GMRES-DR(50,30), i.e., the subspace is 50-dimensional and includes 30 approximate eigenvectors. It is compared to the residual norm

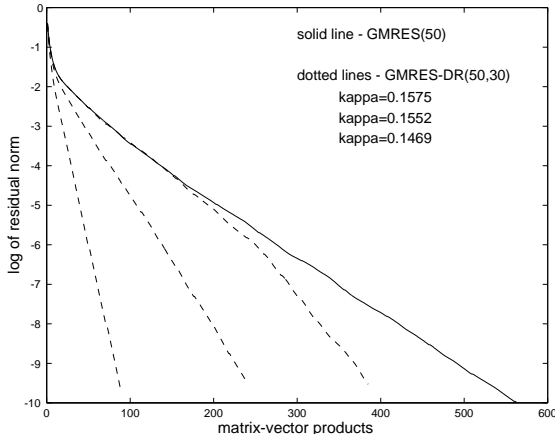


Figure 1. Comparison of the residual norms for standard (unshifted) GMRES(50) (solid magenta) with shifted GMRES-DR(50,30). This is for a $12^3 \times 24$ Wilson-Dirac matrix at $\kappa = 0.1575$ (unshifted), 0.1552, and 0.1469.

for regular GMRES(50). One can see the deflation start to take place around 200 matrix-vector products (the approximate eigenvectors are accurate enough by then).

3. MULTIPLE SHIFTS AND ADDITIONAL RIGHT-HAND SIDES

Typically, many right-hand sides are used to do stochastic estimates of matrix elements. It would be beneficial if the deflated eigenvalues and eigenvectors calculated for the first right-hand side could be reused. Then deflation could begin from the start instead of having to wait for the required eigenvectors to be recalculated, with more dramatic results than in Fig.1. A method to accomplish this called GMRES-Proj was given in [3]. GMRES-Proj alternates cycles of GMRES with projections over the approximate eigenvectors. Next we consider using this for the case of multiple shifts for each of the multiple right-hand sides.

GMRES-DR can deflate eigenvalues and handle multiple shifts at the same time for the first right-hand side (the right-hand sides for each

shifted system can be kept parallel). However, for the second and subsequent right-hand sides there is no way to deflate eigenvalues by projecting over the previously computed approximate eigenvectors and still keep the right-hand sides for the different shifted systems parallel. If the eigenvectors were exact, this would be possible. So one approach is to use only fairly accurate approximate eigenvectors and do a correcting iteration at the end for each shifted system separately.

We now propose a better fix for this problem which does not require accurate eigenvectors. GMRES-DR produces approximate eigenvectors that are represented in the form of an Arnoldi-like recurrence relation:

$$AV_k = V_{k+1}\bar{H}_k, \quad (2)$$

where the columns of V_k span the space of approximate eigenvectors, V_{k+1} has one extra column added to V_k , and \bar{H}_k is a $(k+1)$ by k matrix. Using this, we can perform the projection over the approximate eigenvectors so that the right-hand sides for the different shifted systems are all multiples of each other, except for error in the direction of v_{k+1} , the last column of V_{k+1} . This error can be easily corrected at the end, if we are willing to solve one additional right-hand side, namely v_{k+1} .

There is also potential to develop a deflated version of BiCGStab for multiply shifted systems using this idea. This will be reported later, but for now we will look at deflating BiCGStab for multiple right-hand sides in the non-shifted case.

4. DEFLATED BICGSTAB

The deflation on the additional right-hand sides can employ other methods after the initial eigenvalue generation by GMRES-DR. We have looked at BiCGStab, a non restarted method popular in the lattice community, in this context. We again combine a projection over approximate eigenvectors with the iterative method. However, the projection can only be performed once before the BiCGStab iteration begins. Therefore this projection must reduce the critical eigencomponents to a low enough level that no further reduction is needed during the BiCGStab iteration. The min-

imal residual projection is the best possible one in the sense that it minimizes the norm of the residual vector. However, it can be shown that even if one knows the exact eigenvectors, the corresponding component in the residual vector will not generally be zeroed out (unless the matrix is Hermitian). To deal with this problem, we will give a projection that is better for this task. It uses both left and right approximate eigenvectors.

Left-right Projection for deflating eigenvectors:

1. Let the current approximate solution be x_0 and the current system of equations be $A(x - x_0) = r_0$. Let V be orthonormal with columns spanning the subspace of approximate right eigenvectors. Let U similarly be orthonormal with columns from approximate left eigenvectors.

2. Solve $U^\dagger AVd = c$, where $c = U^\dagger r_0$.

3. The new approximate solution is $x_k = x_0 + Vd$.

This projection can reduce the small eigenvector components better than minimum residual and in the case of exact left and right eigenvectors, the components can be zeroed out. Of course, it is necessary to compute left eigenvectors. However, for many lattice problems, including the Wilson-Dirac matrix, there is a simple relationship between the left and right eigenvectors.

Fig.2 above shows a run on a smaller 4^4 lattice (using MATLAB) of the deflated BiCGStab algorithm using eigenvectors calculated from an initial GMRES-DR solution of the first right-hand side. The deflated solutions take a smaller number of iterations than the nondeflated implementation. Notice that deflation does not care about the nature of the right-hand sides used, so these may be noise vectors or units vectors, as one desires. This applies to all techniques used.

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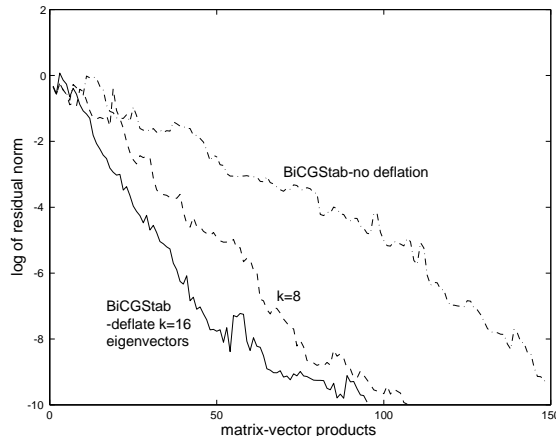


Figure 2. Comparison of standard nondeflated BiCGStab with deflated versions using either 8 or 16 eigenvectors from the initial GMRES-DR run.

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