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Further Improvements in Nonsymmetric Hybrid Iterative Methods

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Abstract

In the past few years new methods have been proposed that can be seen as combinations of standard Krylov subspace methods, such as Bi–CG and GMRES. Such hybrid schemes include CGS, BiCGSTAB, QMRS, TFQMR, and the nested GMRESR method. These methods have been successful in solving relevant sparse nonsymmetric linear systems, but there is still a need for further improvements. In this paper we will highlight some of the recent advancements in the search for effective iterative solvers.

1. Bi-CGSTAB and variants

The residual $r_k = b - Ax_k$ in the Bi-Conjugate Gradient method, when applied to $Ax = b$ with start x_0, can be written formally as $P_k(A)r_0$, where P_k is a k-degree polynomial. These residuals are constructed with one operation with A and one with A^T per iteration step. It was pointed out in [6] that with about the same amount of computational effort one can construct residuals of the form $\tilde{r}_k = P_k^2(A)r_0$, which is the basis for the CGS method.
In [7] it was shown that by a similar approach as for CGS, one can construct methods for which r_k can be interpreted as $r_k = P_k(A)Q_k(A)r_0$, in which P_k is the polynomial associated with BiCG and Q_k can be selected free under the condition that $Q_k(0) = 1$. In [7] it was suggested to construct Q_k as the product of k linear factors $1 - \omega_j A$, where ω_j was taken to minimize locally a residual. This approach leads to the BiCGSTAB method. One weak point in BiCGSTAB is that we get break-down if an ω_j is equal to zero. One may equally expect negative effects when ω_j is small. In fact, BiCGSTAB can be viewed as the combined effect of BiCG and GMRES(1) steps. As soon as the GMRES(1) part of the algorithm (nearly) stagnates, then the BiCG part in the next iteration step cannot (or only poorly) be constructed.
Another dubious aspect of BiCGSTAB is that the factor Q_k has only real roots by construction. It is well-known that optimal reduction polynomials for matrices with complex eigenvalues may have complex roots as well.
This point of view was taken in [2] for the construction of the BiCGSTAB2 method. In the odd-numbered iteration steps the Q-polynomial is expanded by a linear factor, as in BiCGSTAB, but in the even-numbered steps this linear factor is discarded, and the Q-polynomial from the previous even-numbered step is expanded by a quadratic $1 - \omega_j^{(1)}A - \omega_j^{(2)}A^2$. It was anticipated that the introduction of quadratic factors in Q

might help to improve convergence for systems with complex eigenvalues, and, indeed, some improvement was observed in practical situations (see also [3]).
However, our presentation suggests a possible weakness in the construction of BiCGSTAB2, namely in the odd-numbered steps the same problems may occur as in BiCGSTAB. Since the even-numbered steps rely on the results of the odd-numbered steps, this may equally lead to unnecessary break-downs or poor convergence. In [5] another and even simpler approach was taken to arrive at the desired even-numbered steps, without the necessity of the construction of the intermediate BiCGSTAB-type step in the odd-numbered steps. Hence, in this approach the polynomial Q is constructed straight-away as a product of quadratic factors, without ever constructing a linear factor. As a result the new method BiCGSTAB(2) leads only to significant residuals in the even-numbered steps and the odd-numbered steps do not lead necessarily to useful approximations.
In fact, it is shown in [5] that the polynomial Q can also be constructed as the product of ℓ-degree factors, without the construction of the intermediate lower degree factors. The main idea is that ℓ successive BiCG steps are carried out, where for the sake of an A^T-free construction the already available part of Q is expanded by simple powers of A. This means that after the BICG part of the algorithm vectors from the Krylov subspace $s, As, A^2s, ..., A^\ell s$, with $s = P_k(A)Q_{k-\ell}(A)r_0$ are available, and it is then relatively easy to minimize the residual over that particular Krylov subspace. In most cases BiCGSTAB(2) will already give nice results for problems where BiCGSTAB or BiCGSTAB2 may fail.
Bi-CGSTAB(2) can be represented by the following algorithm:

x_0 is an initial guess; $r_0 = b - Ax_0$;
$\hat{r}_0$ is an arbitrary vector, such that $(r, \hat{r}_0) \neq 0$,
    e.g., $\hat{r}_0 = r$;
$\rho_0 = 1; u = 0; \alpha = 0; \omega_2 = 1$;
for $i = 0, 2, 4, 6, ...$
    $\rho_0 = -\omega_2 \rho_0$
even BiCG step:
    $\rho_1 = (\hat{r}_0, r_i); \beta = \alpha\rho_1/\rho_0; \rho_0 = \rho_1$
    $u = r_i - \beta u$;
    $v = Au$
    $\gamma = (v, \hat{r}_0); \alpha = \rho_0/\gamma$;
    $r = r_i - \alpha v$;
    $s = Ar$
    $x = x_i + \alpha u$;
odd BiCG step:
    $\rho_1 = (\hat{r}_0, s); \beta = \alpha\rho_1/\rho_0; \rho_0 = \rho_1$
    $v = s - \beta v$;
    $w = Av$
    $\gamma = (w, \hat{r}_0); \alpha = \rho_0/\gamma$;
    $u = r - \beta u$
    $r = r - \alpha v$
    $s = s - \alpha w$
    $t = As$
GCR(2)-part:
    $\omega_1 = (r, s); \mu = (s, s); \nu = (s, t); \tau = (t, t)$;
    $\omega_2 = (r, t); \tau = \tau - \nu^2/\mu; \omega_2 = (\omega_2 - \nu\omega_1/\mu)/\tau$;
    $\omega_1 = (\omega_1 - \nu\omega_2)/\mu$
    $x_{i+2} = x + \omega_1 r + \omega_2 s + \alpha u$
    $r_{i+2} = r - \omega_1 s - \omega_2 t$
    if x_{i+2} accurate enough then quit
    $u = u - \omega_1 v - \omega_2 w$
end

For more general BiCGSTAB(ℓ) schemes see [5].
Another advantage of BiCGSTAB(2) over BiCGSTAB2 is in its efficiency. The BiCGSTAB(2) algorithm requires 14 vector updates, 9 innerproducts and 4 matrix vector products per full cycle. This has to be compared with a combined odd-numbered and even-numbered step in BiCGSTAB2, which requires 22 vector updates, 11 innerproducts, and 4 matrix vector products, and with two steps of BiCGSTAB which require 4 matrix vector products, 8 innerproducts and 12 vector updates. The numbers for BiCGSTAB2 are based on an implementation described in [3].
Also with respect to memory requirements, BiCGSTAB(2) takes an intermediate position: it requires 2 n-vectors more than BiCGSTAB and 2 n-vectors less than BiCGSTAB2.

2. GMRES in combination with BiCGSTAB

In [8] it is shown how the GMRES-method [4] can be combined (or rather preconditioned) with other iterative schemes. The iteration steps of GMRES (or GCR) are called outer iteration steps, while the iteration steps of the preconditioning iterative method are referred to as inner iterations. The combined method is called GMRES$\star$, where $\star$ stands for any given iterative scheme; in the case of GMRES as the inner iteration method, the combined scheme is called GMRESR in [8].

The GMRES$\star$ algorithm can be described by the following computational scheme:

x_0 is an initial guess; $r_0 = b - Ax_0$;
for $i = 0, 1, 2, 3, \ldots$
  Let $z^{(m)}$ be the approximate solution of $Az = r_i$
  obtained after m steps of an iterative method.
  $c = Az^{(m)}$ (often available from the iterative method)
  for $k = 0, \ldots, i-1$
    $\alpha = (c_k, c)$
    $c = c - \alpha c_k$
    $z^{(m)} = z^{(m)} - \alpha u_k$
  $c_i = c/\|c\|_2$; $u_i = z^{(m)}/\|c\|_2$
  $x_{i+1} = x_i + (c_i, r_i)u_i$
  $r_{i+1} = r_i - (c_i, r_i)c_i$
  if x_{i+1} is accurate enough then quit
end

A sufficient condition to avoid break-down in this method ($\|c\|_2 = 0$) is that the norm of the residual at the end of an inner iteration is smaller than the right-hand residual: $\|Az^{(m)} - r_i\|_2 < \|r_i\|_2$. This can easily be controlled during the inner iteration process. If stagnation occurs, i.e. no progress at all is made in the inner iteration, then it is suggested in [8] to do one (or more) steps of the LSQR method, which guarantees a reduction (but this reduction is often only small).

The idea behind this combined iteration scheme is that we explore parts of high-dimensional Krylov subspaces, hopefully localizing the same approximate solution that full GMRES would find over the entire subspace, but now at much lower computational costs. The alternatives for the inner iteration could be either one cycle of GMRES(m), since then we have also locally an optimal method, or some other iteration scheme, like for instance BiCGSTAB. There are many situations in which we have slow convergence for GMRES(m). In such cases it does not seem wise to use this method.

On the other hand it may also seem questionable whether a method like BiCGSTAB should lead to success in the inner iteration. This method does not satisfy a useful global minimization property and large part of its effectiveness comes from the underlying BiCG algorithm, which is based on bi-orthogonality relations.
In [1] it is proposed to prevent the outer search directions explicitly from being reinvestigated again in the inner process. This is done by keeping the Krylov subspace that is build in the inner iteration orthogonal with respect to the Krylov basis vectors generated in the outer iteration. The procedure works as follows.
In the outer iteration process the vectors c_0, ..., c_{i-1} build an orthogonal basis for the Krylov subspace. Let C_i be the n by i matrix with columns c_0, ..., c_{i-1}. Then the inner iteration process at outer iteration i is carried out with the operator A_i instead of A, and A_i is defined as

$$A_i = (I - C_i C_i^T)A. \tag{1}$$

Of course, this orthogonalization approach for the inner iterations should only be considered in cases where we see too little residual reducing effect in the inner iteration process in comparison to the outer iterations of GMRES$\star$.

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