Analysis of Augmented Krylov Subspace Methods

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Abstract

Residual norm estimates are derived for a general class of methods based on projection techniques on subspaces of the form $K_m + \mathcal{W}$, where K_m is the standard Krylov subspace associated with the original linear system, and $\mathcal{W}$ is some other subspace. These 'augmented Krylov subspace methods' include eigenvalue deflation techniques as well as block-Krylov methods. Residual bounds are established which suggest a convergence rate similar to one obtained by removing the components of the initial residual vector associated with the eigenvalues closest to zero. Both the symmetric and nonsymmetric case are analyzed.

1 Introduction

It has been recently observed that significant improvements in convergence rates can be achieved from Krylov subspace methods by enriching these subspaces in a number of different ways, see, e.g., [2, 4, 8, 9]. One of the simplest ideas employed is to add to the Krylov subspace some approximation to an invariant subspace associated with a few of the lowest eigenvalues. A projection process on this augmented subspace is then carried out. An older technique is to augment the original subspace with other Krylov subspaces, typically with the same matrix and randomly generated right-hand sides. This gives rise to the class of block-Krylov and successive right-hand side methods which have recently seen a regain of interest. [14, 11, 1, 6, 5]. Results of experiments obtained from these alternatives indicate that the improvement in convergence over standard Krylov subspaces of the same dimension can sometimes be substantial. This is especially true when the convergence of the original scheme is hampered by a small number of eigenvalues near zero, see e.g., [2, 9].

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In this paper we take a theoretical look at this general class of 'augmented Krylov methods'. In short, an augmented Krylov method for solving the linear system

$$Ax = b \tag{1}$$

is any projection method in which the subspace of projection is of the form,

$$K = K_m + \mathcal{W}$$

where K_m is the standard Krylov subspace,

$$K_m = \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$$

with $r_0 = b - Ax_0$, the vector x_0 being an arbitrary initial guess to the above linear system. Thus, the usual Krylov subspace K_m, which we sometimes call the primary subspace, is augmented by another subspace $\mathcal{W}$. The intuitive rationale for these methods is that K_m cannot always capture all the 'frequencies' of A, so it may become necessary to include explicitly those components which cause the method to slow-down. There are many possible ways in which to choose the subspace $\mathcal{W}$ following this intuitive idea. In deflation techniques [9, 2], $\mathcal{W}$ is an approximate invariant subspace typically associated with the smallest eigenvalues and obtained as a by-product of earlier projection steps. In block-Krylov techniques, $\mathcal{W}$ consists of the sum (in the linear algebra sense) of a few other Krylov subspaces generated with the same matrix A, but different initial residuals.

We now give a brief background and define some terminology. In what follows, $\mathbb{P}_k$ denotes the space of polynomials of degree not exceeding k, while $\mathbb{P}_k^*$ is the space of polynomials p of degree $\leq k$ normalized so that $p(0) = 1$. An invariant subspace is any subspace X of $\mathbb{C}^n$ such that AX is included in X. If $W = [w_1, \ldots, w_p]$ is a basis of X then X is invariant iff there is a $p \times p$ matrix G such that $AW = WG$. In this paper we often use projections of vectors onto invariant subspaces. This can be done in several ways. Two important options are to use either orthogonal projectors onto the invariant subspace, or spectral projectors. A spectral projector is best defined through the Jordan canonical form. As is well-known, the Jordan canonical form decomposes the subspace $\mathbb{C}^n$ into the direct sum,

$$\mathbb{C}^n = X_1 \oplus X_2 \oplus \cdots \oplus X_l$$

in which each X_i is the invariant subspace associated with a distinct eigenvalue. This direct sum defines canonically a set of l projectors. Each of these projectors maps an arbitrary vector x into its component x_i in the above decomposition. A spectral projector is the sum of any number of these canonical projectors.

Two types of methods are often used to compute an approximate solution from a given subspace. An orthogonal projection method, or orthogonal residual (Orth-res) method extracts an approximation solution of the form $x = x_0 + \delta$ where δ is in K, by imposing the orthogonality constraint: $b - Ax \perp K$. A minimal residual (Min-res) approach computes an approximation in the same form but extracts the approximation by imposing the optimality condition that $\|b - Ax\|_2$ be minimal. This second condition is mathematically equivalent to the orthogonality condition that $b - Ax \perp AK$.

2 Augmented Krylov Methods and FGMRES

To obtain an orthogonal basis of an augmented Krylov subspace, a slight modification of the standard Arnoldi algorithm is needed. Assume that we have a subspace spanned by $m+p$ vectors. Specifically, the first m of these vectors are standard Krylov vectors $v_1, \ldots, v_m$, and the last ones, denoted by $w_1, \ldots, w_s$ form a basis of the additional subspace $\mathcal{W}$. Then at step $m+1$ we introduce the first basis vector w_1 of $\mathcal{W}$, multiply it by A as in the Arnoldi process, and orthogonalize the result against all previous vectors. We then similarly introduce the next basis vector to the subspace and repeat this process. The algorithm is as follows.

ALGORITHM **2.1** *Augmented Arnoldi-Modified Gram-Schmidt*

1. *Choose a vector* v_1 *of norm 1.*
2. *For* $j = 1, 2, \ldots, m+p$ *Do:*
3.   *If* $j \leq m$ *then* $w := Av_j$, *Else* $w := Aw_{j-m}$
4.   *For* $i = 1, \ldots, j$ *do:*
5. $h_{ij} = (w, v_i)$
6. $w := w - h_{ij} v_i$
7.   *EndDo*
9. $h_{j+1,j} = \|w\|_2$. *If* $h_{j+1,j} = 0$ *then Stop.*
10. $v_{j+1} = w / h_{j+1,j}$
11. *EndDo*

We can think of many possible variations to the above basic scheme. For example, the input vectors w_i can themselves be the Krylov vectors of some iterative procedure for solving $Aw = v_{m+1}$. We can also generate another Krylov sequence starting with an arbitrary vector w_1 and append the resulting vectors $w_2, \ldots, w_s$ to the subspace. Some of these variations are explored in [2].

The above algorithm is a trivial extension of the modified Arnoldi process used in the Flexible GMRES (FGMRES) algorithm [12]. Its result is that the vectors $v_1, \ldots, v_{m+p+1}$ forms an orthonormal set of vectors. A number of immediate properties can be established. First the vectors produced by the algorithm satisfy the relation:

$$AZ_{m+p} = V_{m+p+1} \bar{H}_m$$

in which:

$$Z_{m+p} = [v_1, v_2, \ldots, v_m, w_1, w_2, \ldots w_p] \,, \qquad V_{m+p+1} = [v_1, v_2, \ldots, v_{m+p+1}]$$

and $\bar{H}_m$ is the $(m+p+1) \times (m+p)$ upper Hessenberg matrix whose nonzero elements h_{ij} are defined in the algorithm. To solve a linear system with an FGMRES-like approach, we only need to exploit the above relation and the orthogonality of the v_i's. Thus, if $\beta := \|r_0\|_2$ and we start the Arnoldi process with $v_1 := r_0/\beta$, then an approximate solution x from the affine space $x_0 + span\{Z_{m+p}\}$ can be written in the form $x_0 + Z_{m+p}y$ and its residual vector is given by

$$b - Ax = r_0 - AZ_{m+p}y = V_{m+p+1}[\beta e_1 - \bar{H}_m y] \ .$$

Because of the orthogonality of the column-vectors of V_{m+p+1}, the 2-norm of this residual vector can be minimized by solving the least-squares problem $\min_y \|\beta e_1 - \bar{H}_m y\|_2$.

Another important property is that if any vector w in $\mathcal{W}$ is the solution of an equation $Aw = v_i$, for any of the v_i's $i \leq m+1$ then, in general, the exact solution can be extracted from the whole subspace by an FGMRES procedure.

Proposition 2.1 *If there exists a vector w in $\mathcal{W}$ such that $Aw = v_{i+1}$ for some i, $1 \leq i \leq m$ and if the matrix H_i is nonsingular then the affine space $x_0 + K_m + \mathcal{W}$ contains an exact solution to the linear system $Ax = b$.*

Proof. Assume that w is a vector in $\mathcal{W}$ such that $Aw = v_{i+1}$. Recall the standard relation [13],

$$AV_i = V_i H_i + h_{i+1,i} v_{i+1} e_i^T \ . \tag{2}$$

A solution among vectors of the form

$$x = x_0 + V_i y + \alpha w$$

will be constructed. For such vectors the residual $b - Ax$ is given by,

$$r_0 - AV_i y - \alpha A w = V_i \left(\beta e_1 - H_i y\right) - (h_{i+1,i} e_i^T y + \alpha) v_{i+1} \ .$$

If H_i is nonsingular, then y can be chosen so that the 1st term in the right-hand-side vanishes. The scalar α can then be selected to be equal to $-h_{i+1,i} e_i^T y$ to make the second term equal to zero. ∎

In the situation of the proposition, FGMRES will compute the exact solution. That is because FGMRES extracts the (unique) approximate solution with minimum residual. In fact, any projection procedure onto the subspace $x_0 + K_m + \mathcal{W}$ will extract this exact solution because a solution with zero residual can be obtained from the subspace and therefore the Galerkin condition will always be satisfied for this (exact) solution. Note that the proposition is also trivially true for $i = 0$, with the exception that we no longer need the assumption on H_i which does not exist. In addition, it can also be generalized to the situation where there is a vector w in $\mathcal{W}$ such that $Aw = v$ for some vector v in K_{m+1}.

The proposition suggests that a good way to enrich the subspace K_m is to add to it vectors $w_1, \ldots, w_p$ that are approximate solutions of the linear system $Aw = v_i$ for $i \leq m + 1$. These linear systems can be solved with a different preconditioner, for example, one which complements the initial one used for the primary linear system being solved. In effect, we can view this as a multirate approach. The Krylov subspace

K_m is often unable to resolve components of the residual vector that are located in some subspace. Roughly speaking, much of the work in solving the linear system is already accomplished by the subspace K_m. The additional subspace will then fine-tune the current solution in the areas of the spectrum which are not well represented by K_m. In the simplest case, one can add solutions of linear systems $Aw = v_{m+1}$ by another iteration method such as a multi-step SOR. An interesting idea which has been quite successful is to take $\mathcal{W}$ to be an approximate invariant subspace associated with small eigenvalues.

3 Augmenting with Nearly Invariant Subspaces

In what follows we denote by x_0 the initial guess used in the augmented GMRES process for solving the linear system (1), by r_0 the associated initial residual $b - Ax_0$, and by K_m the Krylov subspace

$$K_m(A, r_0) \; = \; \text{Span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\} \; .$$

We make the assumption that there exists an invariant subspace which is close to $\mathcal{W}$ and analyze the behavior of the resulting augmented Krylov subspace algorithm. Our goal is to show a residual bound indicating faster convergence when the invariant subspace is very close to $\mathcal{W}$.

3.1 Basic Results

We recall the following definition of the 'gap' between subspaces. For details on this definition and some properties, see Kato [7] and Chatelin [3].

Definition 3.1 *For any pair of subspaces of* $\mathbb{C}^n$ *define*

$$\delta(X, Y) \; = \; \max_{x \,\in\, X,\; x \neq 0} \; \min_{y \,\in\, Y} \; \frac{\|x - y\|_2}{\|x\|_2} \; . \tag{3}$$

Then, the gap between the subspaces X *and* Y *is,*

$$\Theta(X, Y) = \max\left[\delta(X, Y), \delta(Y, X)\right] \; . \tag{4}$$

Thus, $\delta(X, Y)$ represents the sine of the largest possible angle between vectors in X and their projections in Y. It is worth pointing out that $\delta(X, Y) \; = \|(I - P_Y)P_X\|_2$ in which P_X (resp. P_Y) is an orthogonal projector onto X (resp. Y). In fact when the two subspaces X and Y are of the same dimension then, [3, 7]

$$\Theta(X, Y) = \delta(X, Y) = \delta(Y, X) = \|P_X - P_Y\|_2 \; .$$

In this case, $\Theta(X, Y)$ can be viewed as the sine of the angle between the two subspaces X and Y.

Theorem 3.1 *Assume that a minimal residual projection method is applied to A using the augmented Krylov subspace,*

$$K = K_m \; + \; \mathcal{W} \; ,$$

in which the subspace $A\mathcal{W}$ is at a gap of ϵ from a certain invariant subspace U, i.e., there exists an invariant subspace U, such that

$$\Theta(U, A\mathcal{W}) = \epsilon \; .$$

Let P_U be any projector onto U. Then the residual $\tilde{r}$ obtained from the minimal residual projection process onto the augmented Krylov subspace K satisfies the inequality,

$$\|\tilde{r}\|_2 \leq \min_{q \,\in\, \mathbb{P}^*_m} \{ \; \|q(A)(I - P_U)r_0\|_2 + \epsilon \; \|q(A)P_U r_0\|_2\} \; .$$

Proof. By definition, we have

$$\begin{aligned} \|\tilde{r}\|_2 &= \min_{z \,\in\, K_m + \mathcal{W}} \|r_0 - Az\|_2 && (5)\\ &= \min_{v \,\in K_m, w \in \mathcal{W}} \|(r_0 - Av) - Aw\|_2 \; . && (6) \end{aligned}$$

Each vector v in K_m is of the form $v = s(A)r_0$ where s is a polynomial of degree $\leq m-1$. It results that the vector $r_0 - Av$ is of the form $q(A)r_0$ where q belongs to the space of polynomials in $\mathbb{P}$ which satisfy the constraint $q(0) = 1$. Hence,

$$\begin{aligned} \|\tilde{r}\|_2 &= \min_{q \,\in\, \mathbb{P}^*_m;\; w \,\in\, \mathcal{W}} \|q(A)r_0 - Aw\|_2 \\ &= \min_{q \,\in\, \mathbb{P}^*_m;\; w \,\in\, \mathcal{W}} \|q(A)(I - P_U)r_0 + q(A)P_U r_0 - Aw\|_2 && (7)\\ &\leq \min_{q \,\in\, \mathbb{P}^*_m;\; w \,\in\, \mathcal{W}} \|q(A)(I - P_U)r_0\|_2 + \|q(A)P_U r_0 - Aw\|_2 \; . && (8) \end{aligned}$$

Observing that $q(A)P_U r_0$ belongs to the subspace U, the second term on the right-hand-side of (8) is bounded from above by $\epsilon\|q(A)P_U r_0\|_2$ and this completes the proof. ■

The above theorem can be exploited in many different ways. In particular, we may obtain different bounds depending on which type of projector P_U is used. For example, assume that P_U is the spectral projector associated with a set of eigenvalues $\lambda_1, \ldots, \lambda_s$, with $s \leq p$. Let q^*_m be the optimal GMRES polynomial obtained for the deflated initial residual $r_d = (I - P_U)r_0$:

$$\|q^*_m(A)r_d\|_2 = \min_{q \in \; \mathbb{P}^*_m} \|q(A)r_d\|_2 \; .$$

Denote by $\tilde{r}_d = q^*_m(A)r_d$ the GMRES residual vector achieved on this linear system. Then applying the theorem, we immediately get

$$\begin{aligned} \|\tilde{r}\|_2 &\leq \|q^*_m(A)r_d\|_2 + \epsilon \; \|q^*_m(A)P_U r_0\|_2 \\ &= \|\tilde{r}_d\|_2 + \epsilon \; \|q^*_m(A)P_U r_0\|_2 \; . \end{aligned}$$

The first term in the right-hand-side is the result of m steps of a GMRES iteration used to solve the deflated linear system,

$$Ax = (I - P_U)r_0$$

starting with a zero initial guess. If A is diagonalizable and if the initial residual has the expansion $\sum \alpha_i u_i$ the second term $q_m^*(A)P_U r_0$ will have components $q_m^*(\lambda_i)u_i\alpha_i$ in the eigenbasis. For those eigenvalues close to zero, $q_m^*(\lambda_i)$ should be close to one since $q_m^*(0) = 1$. If U is associated with eigenvalues close to zero, and if ϵ is small we can therefore expect the method to behave essentially like a deflated GMRES procedure, i.e., a procedure in which the initial residual is stripped off of all the components associated with the subspace U. In fact if $\mathcal{W}$ is exactly invariant then $\epsilon = 0$ and $\|\tilde{r}\|_2 \leq \|r_d\|_2$, so we should expect the method to behave like a deflated GMRES procedure in this case. We remark that the result of the theorem can be slightly improved by replacing the subspace $\mathcal{W}$ in the minimum (7) by the whole subspace K. This can be easily seen from Equation (6).

An immediate corollary of the theorem is the following.

Corollary 3.1 *Let P_U be a projector into the invariant subspace U and let the assumption of Theorem 3.1 be satisfied. Also assume that there is a polynomial q in $\mathbb{P}_m^*$ such that,*

$$\begin{aligned} \|q(A)(I - P_U)r_0\|_2 &\leq s_m \|(I - P_U)r_0\|_2 & (9) \\ \|q(A)P_U r_0\|_2 &\leq c_m \|P_U r_0\|_2 & (10) \end{aligned}$$

Then the residual $\tilde{r}$ obtained from the minimal residual projection process onto the augmented Krylov subspace K satisfies the inequality,

$$\|\tilde{r}\|_2 \leq s_m \|(I - P_U)r_0\|_2 + \epsilon c_m \|P_U r_0\|_2 \ , \tag{11}$$

and in the case when P_U is an orthogonal projector,

$$\|\tilde{r}\|_2 \leq \sqrt{s_m^2 + \epsilon^2 c_m^2} \ \|r_0\|_2 \ . \tag{12}$$

The second part of the corollary follows by applying the Cauchy-Schwarz inequality to (11).

At this point we might provide error bounds using an eigenvector expansion of the initial residual and exploiting standard approximation theory results based on Chebyshev polynomials. These would give upper bounds for s_m and c_m from some knowledge on the spectrum of the matrix. However, these bounds would utilize in one way or another the condition number of the matrix of eigenvectors which can be very large in case A is highly nonnormal. Therefore, this is considered only for the Hermitian case to be seen shortly. For the non-Hermitian case, we will instead consider the problem from a different angle and attempt to compare the result of the process with that of a GMRES iteration which is expected to converge faster. This is taken up in the next section.

3.2 Comparison results

A desirable result to state would be that the augmented Krylov subspace method converges similarly to the GMRES algorithm applied to the deflated linear system $A\delta = r_d$. Here, the deflated residual r_d is obtained from the residual vector r_0 by removing all components in the subspace $\mathcal{W}$. In the case when $\mathcal{W}$ is an exact invariant space this turns out to be true, as was indicated above. If it is only close to an invariant subspace, then, an intermediate result is to be expected.

Corollary 3.2 *Let $\bar{r}$ be the residual obtained from m steps of GMRES applied to the $2n \times 2n$ linear system,*

$$\begin{pmatrix} A & O \\ O & A \end{pmatrix} \begin{pmatrix} \delta_1 \\ \delta_2 \end{pmatrix} = \begin{pmatrix} \epsilon P_U r_0 \\ (I - P_U) r_0 \end{pmatrix} \tag{13}$$

starting with a zero initial guess. Then the residual $\tilde{r}$ obtained from the minimal residual projection process onto the augmented Krylov subspace K satisfies the inequality,

$$\|\tilde{r}\|_2 \leq \sqrt{2}\ \|\bar{r}\|_2 \ .$$

Proof. Denote by B and $\bar{r}_0$ the matrix and right-hand side of the linear system (13). As is well-known, the GMRES algorithm applied to the system (13) with zero initial guess minimizes the 2-norm $\|q(B)\bar{r}_0\|_2$ over all polynomials in $\mathbb{P}_m^*$. Let $\bar{q}$ be the polynomial which achieves this minimum. We then have

$$\begin{aligned} \|\bar{r}\|_2 &= \|\bar{q}(B)\bar{r}_0\|_2 \\ &= \left(\|\bar{q}(A)(I - P_U)r_0\|_2^2 + \|\bar{q}(A)(\epsilon P_U r_0)\|_2^2\right)^{1/2} \\ &= \left(\|\bar{q}(A)(I - P_U)r_0\|_2^2 + \epsilon^2\|\bar{q}(A)P_U r_0\|_2^2\right)^{1/2} \end{aligned} \tag{14}$$

From Theorem 3.1 we can state that

$$\|\tilde{r}\|_2 \leq \ \|\bar{q}(A)(I - P_U)r_0\|_2 + \epsilon\ \|\bar{q}(A)P_U r_0\|_2$$

which gives the result in view of (14) and the inequality $|a| + |b| \leq \sqrt{2}\ \sqrt{a^2 + b^2}$ ∎

In the above result we had to use a linear system of size twice that of the original matrix in order to obtain an inequality using any projector P_U. It is possible to obtain a similar comparison result using a related linear system of size n only, by being more specific about the projector P_U. However, in this case, the inequality is weakened by the presence of the angle between the invariant subspace U and its complement. The following lemma will be needed.

Lemma 3.1 *Let U and V be any two subspaces and let θ be the acute angle between them as defined by*

$$\cos\theta \ = \ \max_{u \in U;\ v \in V} \frac{|(u, v)|}{\|u\|_2 \|v\|_2} \ .$$

Then, the following inequality holds for any pair of vectors u, v with u in U and v in V

$$\|u+v\|_2 \geq \sqrt{2}\sin\frac{\theta}{2}\left(\|u\|_2^2+\|v\|_2^2\right)^{1/2} . \tag{15}$$

The proof of the lemma is straightforward and is omitted. If P_U is a spectral projector then it commutes with A and with any polynomial of A. In addition, $I - P_U$ is also a spectral projector which commutes with A as well as with any polynomial $q(A)$. We now show a result similar to that of the previous corollary.

Corollary 3.3 *Let P_U be the spectral projector associated with the invariant subspace U and θ the acute angle between $P_U\mathbb{C}^n$ and $(I-P_U)\mathbb{C}^n$. Let $\bar{r}$ be the residual obtained from m steps of GMRES applied to the linear system,*

$$A\delta = \epsilon P_U r_0 + (I-P_U)r_0 \tag{16}$$

starting with a zero initial guess. Then, the residual $\tilde{r}$ obtained from the minimal residual projection process onto the augmented Krylov subspace K satisfies the inequality,

$$\|\tilde{r}\|_2 \leq \frac{\|\bar{r}\|_2}{\sin\frac{\theta}{2}} .$$

Proof. The GMRES algorithm applied to the system (16) with zero initial guess minimizes the 2-norm $\|q(A)\left(\epsilon P_U r_0 + (I-P_U)r_0\right)\|_2$ over all polynomials q in $\mathbb{P}_m^*$. Let $\bar{q}$ be the polynomial which achieves this minimum. Since $\bar{q}(A)P_U r_0$ belongs to $P_U\mathbb{C}^n$ and $\bar{q}(A)(I-P_U)r_0$ belongs to $(I-P_U)\mathbb{C}^n$ we have by the previous lemma

$$\begin{aligned}\|\bar{r}\|_2 &= \|\bar{q}(A)(I-P_U)r_0 + \bar{q}(A)(\epsilon P_U r_0)\| \\ &\geq \sqrt{2}\sin\frac{\theta}{2}\left(\|\bar{q}(A)(I-P_U)r_0\|_2^2 + \epsilon^2\|\bar{q}(A)P_U r_0\|_2^2\right)^{1/2} .\end{aligned} \tag{17}$$

Theorem 3.1 implies that

$$\|\tilde{r}\|_2 \leq \|\bar{q}(A)(I-P_U)r_0\|_2 + \epsilon\,\|\bar{q}(A)P_U r_0\|_2$$

which gives the result in view of (17) and the inequality $|a|+|b| \leq \sqrt{2}\,\sqrt{a^2+b^2}$ ■
The angle θ is related to conditioning of the invariant subspace U. In the ideal case when $\theta = \pi/2$, then we obtain the same result as that of Corollary 3.2, namely, $\|\tilde{r}\|_2 \leq \sqrt{2}\,\|\bar{r}\|_2$.

3.3 Hermitian case

The results of previous sections can be made more explicit in the particular case when the matrix is symmetric positive definite.

Corollary 3.4 *Assume that A is symmetric positive definite with eigenvalues*

$$\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n ,$$

and let the assumptions of Theorem 3.1 be satisfied, with U being the s-dimensional eigenspace associated with the eigenvalues $\lambda_1, \ldots, \lambda_s$, where $s \leq p$. Then the residual $\tilde{r}$ obtained from the minimal residual projection process onto the augmented Krylov subspace K satisfies the inequality,

$$\|\tilde{r}\|_2 \leq \|r_0\|_2 \sqrt{\frac{1}{T_m^2(\gamma)} + \epsilon^2} \tag{18}$$

in which

$$\gamma \equiv \frac{\lambda_n + \lambda_{s+1}}{\lambda_n - \lambda_{s+1}}$$

and T_m is the Chebyshev polynomial of degree m of the first kind.

Proof. Define

$$\alpha = \frac{2}{\lambda_n - \lambda_{s+1}} , \quad q_m(t) = \frac{T_m(\gamma - \alpha t)}{T_m(\gamma)}$$

Referring to the result of Corollary 3.1 we will obtain upper bounds for the numbers s_m and c_m in the Corollary for the above polynomial q. Assuming that the residual r_0 is expanded in the (orthonormal) eigenbasis as

$$r_0 = \sum_{i=1}^{n} \alpha_i u_i$$

then, we have

$$\|q(A)(I - P_U)r_0\|_2^2 = \frac{1}{T_m(\gamma)^2} \sum_{i>s} T_m(\gamma - \alpha\lambda_i)^2 \alpha_i^2 .$$

By definition of α we have $|\gamma - \alpha\lambda_i| \leq 1$ for $i > s$ and as a result $|T_m(\gamma - \alpha\lambda_i)| \leq 1$. Thus, the above expression is upper bounded by

$$\|q(A)(I - P_U)r_0\|_2^2 \leq \frac{1}{T_m(\gamma)^2} \sum_{i>s} \alpha_i^2 = \frac{\|(I - P_U)r_0\|_2^2}{T_m(\gamma)^2}$$

and so we can define $s_m \equiv 1/T_m(\gamma)$. Similarly, the term $\|q(A)P_U r_0\|_2$ of Corollary 3.1 can be expanded as

$$\|q(A)P_U r_0\|_2^2 = \sum_{i \leq s} (q(\lambda_i)\alpha_i)^2$$

In the interval $[0, \lambda_{s+1}]$ the function $q(\lambda)$ is a decreasing function and is therefore upper bounded by $q(0) = 1$. This yields,

$$\|q(A)P_U r_0\|_2^2 \leq \sum_{i \leq s} \alpha_i^2 = \|P_U r_0\|_2^2.$$

As a result we can define $c_m = 1$. The result follows immediately from Corollary 3.1. ■

4 Case of block-Krylov methods

Results of a slightly different type can be derived for block-Krylov methods. In these methods the subspace of projection is

$$K = K_m^{(1)} + \mathcal{W}$$

with

$$\mathcal{W} = K_m^{(2)} + K_m^{(3)} + \cdots K_m^{(s)} \ ,$$

where $K_m^{(i)} = \text{span}\left[v_1^{(i)}, Av_1^{(i)}, \ldots, A^{m-1}v_1^{(i)}\right]$. The starting vector $v_1^{(1)}$ of the the first Krylov subspace is the normalized residual $r_0/\|r_0\|_2$. A number of results for analyzing block methods have already been established in the literature [10, 14]. The approach presented here shows similar results which are somewhat simpler, by introducing systematically a subsidiary approximate solution obtained by a projection step onto the subspace spanned by the initial block. Results using Chebyshev polynomials are omitted again except in the Hermitian case.

4.1 General results

An important factor in the convergence of block methods is the subspace S spanned by the initial block, i.e., the subspace

$$S = \text{span}\{v_1^{(1)}, v_1^{(2)}, \ldots, v_1^{(s)}\} \ .$$

Consider any subspace U of dimension s. Typically, U will be an invariant subspace associated with the s lowest eigenvalues but this is not required in the analysis which follows. As a background, recall that any projector can be defined with the given of two subspaces, its range M and its null space N. It is common to define N via its orthogonal complement L which has the same dimension s as M. Thus,

$$Range(P) = M; \quad Null(P) = L^{\perp} \ .$$

With P is associated the decomposition of $\mathbb{C}^n$ into the direct sum

$$\mathbb{C}^n = M \oplus L^{\perp} \ . \tag{19}$$

We say that P is a projector *onto* M and *orthogonal* to L. Given two subspaces M and L, each of dimension s, a projector onto M and orthogonal to L can be defined whenever

$$M \cap L^{\perp} = \{0\},$$

which is the condition under which $\mathbb{C}^n$ is the direct sum of the two subspaces M and $L^{\perp}$. Recall also that the projection u of an arbitrary vector x onto M and orthogonal to L is defined by the requirements,

$$u \ \in \ M, \quad x - u \ \perp \ L \ .$$

The first of these requirements defines the s degrees of freedom, and the second defines the s constraints that allow us to extract $u = Px$ given these degrees of freedom. We now establish the following lemma.

Lemma 4.1 *Let P_U be a projector onto a subspace U and orthogonal to a subspace L, and assume that the subspace S satisfies the condition*

$$AS \ \cap L^{\perp} = \{0\} \ . \tag{20}$$

Then, for any vector r in $\mathbb{C}^n$ there exists a unique vector w in $\mathcal{W}$ such that

$$P_U(r - Aw) = 0 \ . \tag{21}$$

The vector Aw is the projection of r onto the subspace AS and orthogonal to L. The vector w is the result of a projection process onto S orthogonally to L for solving the linear system $A\delta = r$, starting with a zero initial guess.

Proof. Under the condition (20) the projector P_{AS} onto AS and orthogonal to L exists, and therefore, for any r there exists a unique Aw in AS, obtaining by projecting r onto AS and orthogonally to L. This Aw satisfies the condition $r - Aw \perp L$ which implies that the vector $r - Aw$ belongs to $null(P_U) = L^{\perp}$ or, equivalently, $P_U(r - Aw) = 0$. The rest of the proof follows from the definitions of projectors and projection methods for linear systems. ■

Condition (21) can be rewritten as

$$Aw = P_U r + (I - P_U)Aw \tag{22}$$

because $Aw = P_U Aw + (I - P_U)Aw$ and (21) implies that $P_U Aw = P_U r$. The above equation means that the vector Aw has the same U-component as r in the direct sum decomposition (19) associated with the projector P_U. Consider the basis

$$V_1 = [v_1^{(1)}, v_1^{(2)}, \ldots, v_1^{(s)}]$$

of S. If A is nonsingular then AV_1 is a basis of AS. Let $Z = [z_1, \ldots, z_s]$ be a basis of L. Then it can be easily seen that condition (20) is equivalent to the nonsingularity of the $s \times s$ matrix $Z^H AS$. The condition (21) immediately yields,

$$w = V_1(Z^H AV_1)^{-1} Z^H r \ .$$

Theorem 4.1 *Let P_U be a projector onto a subspace U of dimension s such that the condition (20) is satisfied for $L = Null(P_U)^{\perp}$. Let w_0 be the vector w defined by Lemma 4.1 for the case when $r \equiv r_0$ and denote by $\hat{r}_0$ the associated residual $\hat{r}_0 = r_0 - Aw_0$. Then the residual $\tilde{r}$ obtained from the minimal residual projection process onto the augmented Krylov subspace K satisfies the inequality,*

$$\|\tilde{r}\|_2 \leq \min_{p \ \in \mathbb{P}_m^*} \|q(A)(I - P_U) \ \hat{r}_0\|_2 \ . \tag{23}$$

Proof. We start similarly to the proof of Theorem 3.1:

$$\begin{aligned}\|\tilde{r}\|_2 &= \min_{z\ \in K=\ K_m+\mathcal{W}} \|r_0 - Az\|_2 \\ &= \min_{v\ \in K_m, w\in K} \|(r_0 - Av) - Aw\|_2\ .\end{aligned}$$

As was seen before, a generic vector $r_0 - Av$ is of the form $q(A)r_0$ where q is a polynomial of degree $\leq m$ such that $q(0) = 1$ and therefore,

$$\begin{aligned}\|\tilde{r}\|_2 &= \min_{q\in\mathbb{P}^*_m,\ w\in K} \|q(A)r_0 - Aw\|_2 \\ &= \min_{q\in\mathbb{P}^*_m, w\in K} \|q(A)(I-P_U)r_0 + q(A)P_U r_0 - Aw\|_2\ .\end{aligned}$$

For any polynomial q in $\mathbb{P}^*_m$ and for any vector w in K we have,

$$\|\tilde{r}\|_2 \leq \|q(A)(I-P_U)r_0 + q(A)P_U r_0 - Aw\|_2\ . \tag{24}$$

Consider now the particular vector $w = q(A)w_0$ where the vector w_0 is defined by the theorem. Using the result of Lemma 4.1, and the equality (22) we obtain,

$$\begin{aligned} q(A)P_U r_0 - Aw &= q(A)P_U r_0 - Aq(A)w_0 \\ &= q(A)P_U r_0 - q(A)Aw_0 \\ &= q(A)P_U r_0 - q(A)[P_U r_0 + (I-P_U)Aw_0] \\ &= -q(A)(I-P_U)Aw_0\ .\end{aligned}$$

Substituting this in Equation (24) for any polynomial q, results in

$$\|\tilde{r}\|_2 \leq \|q(A)(I-P_U)(r_0 - Aw_0)\|_2 \tag{25}$$

Taking the minimum of the right-hand side over all polynomials in $\mathbb{P}^*_m$ yields the desired result. ∎

This simple theorem states that a block-GMRES method will do at least as well as a GMRES method on the linear system whose initial residual has been stripped off the components in the subspace U by a projection process on the initial subspace S. The removal of these undesired components, is achieved by a projection process onto S orthogonally to $L = Null(P_U)^\perp$, as expressed by the Galerkin conditions,

$$w_0\ \in\ S\ , \qquad r_0 - Aw_0 \perp Null(P_U)^\perp\ .$$

Note again that P_U is any projector onto the subspace U.

The projector $I - P_U$ in Equation (23) is not really needed since $\hat{r}_0$ has no components in the subspace U and so $(I-P_U)\hat{r}_0 = \hat{r}_0$. However, its presence is helpful when P_U is a spectral projector, since in this situation,

$$q(A)(I-P_U) = q((I-P_U)A(I-P_U))\ ,$$

showing that the GMRES iteration associated with the minimum in (23) is equivalent to a GMRES iteration for solving a linear system *restricted to the spectral complement of* U.

4.2 Block Krylov methods in the SPD case

We assume throughout this section that A is SPD with the eigenvalues

$$0<\lambda_1 \leq \lambda_2 \cdots \leq \lambda_n \ .$$

Here, the subspace U is chosen to be the invariant subspace associated with the eigenvalues $\lambda_1, \ldots, \lambda_p$ and P_U is the spectral projector associated with U. In this case, P_U is the *orthogonal* projector onto U and the subspace L which was defined as the orthogonal complement of the null space of P becomes equal to U itself.

By selecting the polynomial in Theorem 4.1 carefully a rather simple result can be obtained.

Theorem 4.2 *Let P_U be the orthogonal projector onto the invariant subspace associated with the eigenvalues $\lambda_1, \ldots, \lambda_p$ and assume the condition (20) is satisfied. Let w_0 be the vector w defined by Lemma 4.1 for the case when $r \equiv r_0$ and $\hat{r}_0 = r_0 - Aw_0$. Then the residual $\tilde{r}$ obtained from the minimal residual projection process onto the augmented Krylov subspace K satisfies the inequality,*

$$\|\tilde{r}\|_2 \leq \frac{\|\hat{r}_0\|_2}{T_m(\gamma)} \ . \tag{26}$$

with

$$\gamma \equiv \frac{\lambda_n + \lambda_{p+1}}{\lambda_n - \lambda_{p+1}}$$

Proof. According to Theorem 4.1, for any polynomial q in $\mathbb{P}_m^*$ we have

$$\|\tilde{r}\|_2 \leq \|q(A)(I - P_U)\ \hat{r}_0\|_2 \leq \|q(A)(I - P_U)\|_2\ \|\hat{r}_0\|_2 \ . \tag{27}$$

Since $I - P_U$ is a spectral projector of A we have,

$$q(A)(I - P_U) = (I - P_U)q(A) = (I - P_U)q(A)(I - P_U) \ .$$

The only nonzero eigenvalues of the Hermitian operator $(I - P_U)q(A)(I - P_U)$ are $q(\lambda_i)$ for $i > p$. Thus,

$$\|(I - P_U)q(A)(I - P_U)\|_2 = \max_{i=p+1,\ldots,n} |q(\lambda_i)| \ . \tag{28}$$

Consider the polynomial $q_m(t)$ defined by

$$q_m(t) = \frac{T_m(\gamma - \alpha t)}{T_m(\gamma)}$$

where γ is defined above and

$$\alpha \equiv \frac{2}{\lambda_n - \lambda_{p+1}} \ .$$

Clearly, q_m belongs to $\mathbb{P}_m^*$. In addition, for t in the closed interval $[\lambda_{p+1}, \lambda_n]$, we have $|\gamma - \alpha t| \leq 1$ so that $|T_m(\gamma - \alpha t)| \leq 1$. For this polynomial the norm of the Hermitian operator, $(I - P_U)q(A)(I - P_U)$ in (28) becomes

$$\|q(A)(I - P_U)\|_2 = \|(I - P_U)q(A)(I - P_U)\|_2 = \max_{i=p+1,\ldots,n} |q_m(\lambda_i)| \leq \frac{1}{T_m(\gamma)} \tag{29}$$

Substituting this inequality in (27) yields the desired result. ∎

5 Numerical experiment

The behaviors of the deflated algorithms and the Block-GMRES algorithms are now illustrated on a simple example. Consider a diagonal matrix of size $n = 200$ whose diagonal entries are given by

$$d_i = \begin{cases} \frac{i}{n} & \text{when } i > 4 \\ 0.05 \times \frac{i}{n} & \text{when } i \leq 4 \ . \end{cases}$$

This distribution is chosen to have a small cluster of eigenvalues around the origin. In all tests, the right-hand side b of the linear system is made of (the same) pseudo-random values, and the initial guess taken is the zero vector. Though the matrix is symmetric, nonsymmetric iterative solvers such as GMRES and block-GMRES are used in this experiment. The following runs were made.

1. Standard GMRES without restarts and restarted GMRES, with a Krylov dimension of 40.

2. Block GMRES (BGMRES) without restarts. The block size chosen is four, which is the size of the cluster.

3. A deflated GMRES algorithm as described in [9] and [2]. This consists of adding approximate eigenvectors obtained from the previous Arnoldi step, to the Krylov subspace. The test uses a subspace dimension of 40, the last four of which are approximate eigenvectors (except in the first outer iteration). This is denoted by DGMRES(40,4).

4. For comparison, a run of (nonrestarted) GMRES is shown on the deflated system. This system of dimension 196 has a diagonal coefficient matrix with entries $d_5, d_6, \ldots d_{200}$ and the right-hand side b with components $b_5, \ldots, b_{200}$. A zero initial guess was also used.

In the block-GMRES case, 4 linear systems are actually solved simultaneously, the first of which is the desired linear system. The right-hand sides of the other 3 linear systems are chosen randomly and the associated initial guesses are again zero vectors.

The convergence history for these runs is plotted in Figure 1. As is observed, all curves, except the restarted GMRES curve, have similar convergence slopes towards the final phase of the iteration. The first 40 steps of GMRES, GMRES(40) and DGMRES(40,4) (deflated GMRES) are identical. Differences appear at around step 60, half way into the second outer loop, between full GMRES and the other two methods. GMRES(40) and DGMRES(40,4) are still identical until step 76. Indeed, in the first outer loop, there was no eigenspace information to be fed into DGMRES so a plain restarted GMRES is used. The last four vectors entered into DGMRES are eigenvectors obtained from the first Krylov subspace. Then the behavior of the iteration from that point on is very close to that of the full GMRES and GMRES on the deflated system.

It is interesting to note that in this case the full GMRES algorithm performs best. We must keep in mind that after step 40, the full GMRES iteration uses a subspace which includes the same eigenvectors as DGMRES(40,4). It is therefore able to capture those eigenmodes in the same way as the deflated GMRES as shown by the curves. Also interesting is the observation that the block-GMRES algorithm seems to take longer to capture the cluster and reach the final convergence phase. If we had to solve four simultaneous linear system, the Block-GMRES algorithm would be competitive since it would take an average of 45 steps for each linear system to converge (assuming they converge at roughly equal speed on average). If we had only one linear system to solve, the results of the plot indicate that a plain or a deflated GMRES run may achieve far better performance. This is confirmed by experiments elsewhere, see e.g., [2].

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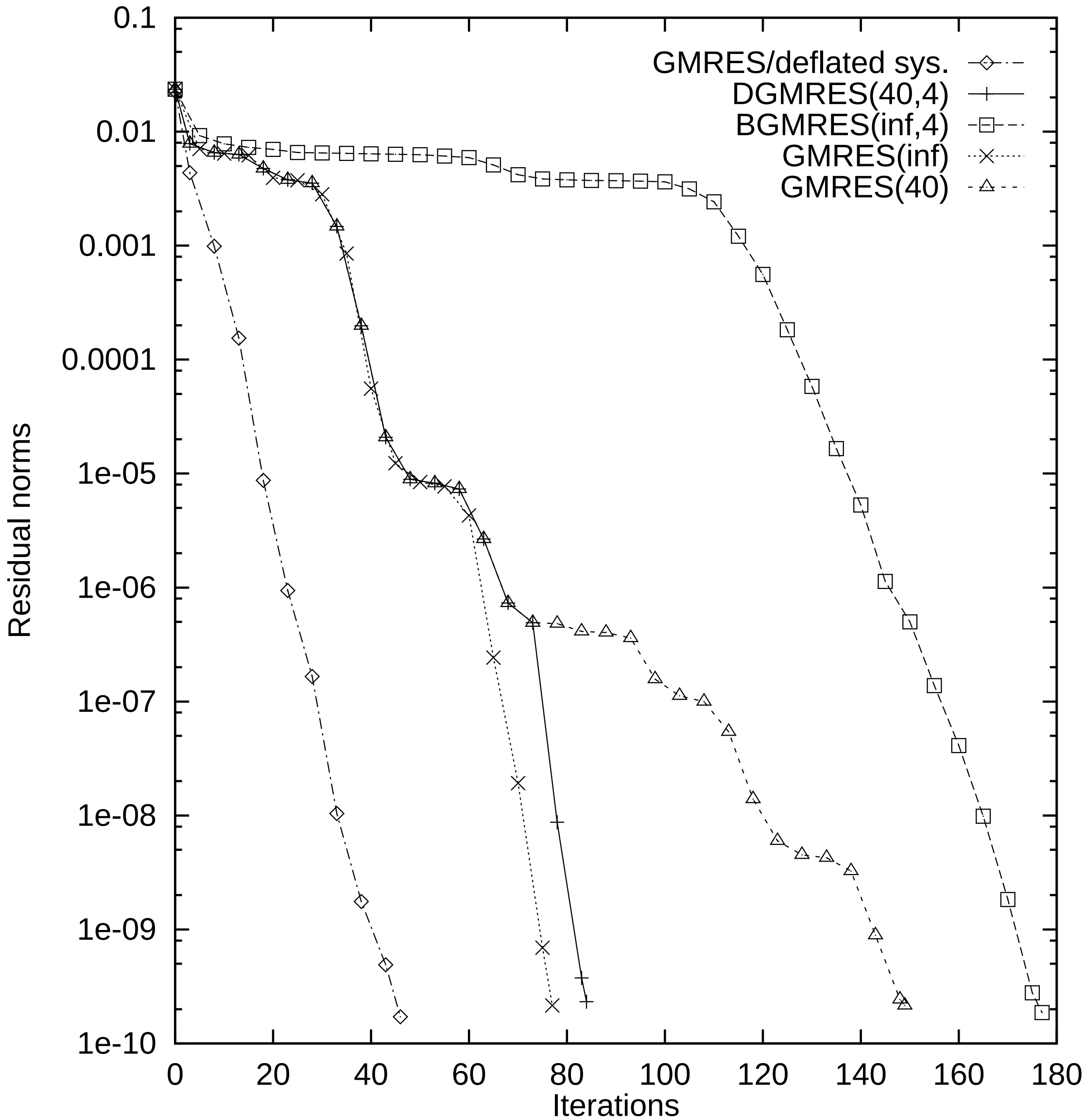

Figure 1: Behavior of GMRES and Block-GMRES on a matrix whose spectrum has a cluster around the origin

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