Improving Eigenvectors in Arnoldi's Method

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July 14, 1995

Abstract

The Ritz vectors obtained by Arnoldi's method may not be good approximations and even may not converge even if the corresponding Ritz values do. In order to improve the quality of Ritz vectors and enhance the efficiency of Arnoldi type algorithms, we propose a strategy that uses Ritz values obtained from an m-dimensional Krylov subspace but chooses modified approximate eigenvectors in an $(m+1)$-dimensional Krylov subspace. Residual norm of each new approximate eigenpair is minimal over the span of the Ritz vector and the $(m+1)$th basis vector, which is *available* when the m-step Arnoldi process is run. The resulting modified m-step Arnoldi method is better than the standard m-step one in theory and cheaper than the standard $(m+1)$-step one. Based on this strategy, we present a modified m-step restarted Arnoldi algorithm. Numerical examples show that the modified m-step restarted algorithm and its version with Chebyshev acceleration are often considerably more efficient than the standard $(m+1)$-step restarted ones.

Key words. Large unsymmetric, the m-step Arnoldi process, the m-step Arnoldi method, eigenvalue, Ritz value, eigenvector, Ritz vector, modified

AMS(MOS) subject classification. 65F15

1 Introduction

Arnoldi's method [1, 11] is suitable for computing a few selected eigenpairs of large unsymmetric matrices. It has been investigated since the 1980s; see, e.g., [3, 4, 6, 7, 8, 9, 10, 12, 13, 14].

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It is well known that the m-step Arnoldi process, as described in detail in Section 2, generates an orthonormal basis $\{v_j\}_{j=1}^m$ of the Krylov subspace $\mathcal{K}_m(v_1, A)$ spanned by $v_1, Av_1, \ldots, A^{m-1}v_1$. Here v_1 is an initial unit norm vector. The projected matrix of A onto $\mathcal{K}_m(v_1, A)$ is represented by an $m \times m$ upper Hessenberg matrix H_m. Then the m-step Arnoldi method uses the Ritz pairs $\lambda^{(m)}, \varphi^{(m)}$ of A in $\mathcal{K}_m(v_1, A)$ to approximate some eigenpairs λ, φ of A.

The convergence analysis in [4, 8, 12] gives a *necessary* condition for the convergence of Arnoldi's method. It states that the distance between the wanted φ and $\mathcal{K}_m(v_1, A)$ must approach zero as m increases. However, it is not *sufficient*, since it is proved in [4, 8] that Ritz vectors $\varphi^{(m)}$ may not be good approximations in theory for a general unsymmetric matrix A even though these distances approach zero and the corresponding $\lambda^{(m)}$ converge. For more details and numerical experiments we refer to [7].

This suggests that we seek new strategies to improve the quality of $\varphi^{(m)}$ and to enhance the efficiency of Arnoldi type algorithms. The first approach is to keep $\lambda^{(m)}$ but *completely discard* $\varphi^{(m)}$. Instead, the refined approximate eigenvector is chosen in $\mathcal{K}_m(v_1, A)$, such that it minimizes the norm of the residual formed with the Ritz value. It can be computed relatively cheaply by solving an $(m+1) \times m$ singular value decomposition problem. It is shown in [7, 8] that the refined vectors converge if the corresponding Ritz values $\lambda^{(m)}$ do, so the possible non-convergence of eigenvectors is ruled out in theory. Numerical experiments have demonstrated that the resulting refined algorithms are much more efficient than the standard counterparts.

In this note, we follow a different approach. We observe that the m-step Arnoldi process generates an orthonormal basis of $\mathcal{K}_{m+1}(v_1, A)$ *rather than* of $\mathcal{K}_m(v_1, A)$, that is, the $(m+1)$th basis vector v_{m+1} of $\mathcal{K}_{m+1}(v_1, A)$ is already *available* when the m-step Arnoldi process is performed. However, although the basis vectors $\{v_j\}_{j=1}^{m+1}$ of $\mathcal{K}_{m+1}(v_1, A)$ are available in this case, we have only obtained the $m \times m$ projected matrix H_m of A onto $\mathcal{K}_m(v_1, A)$. Therefore, v_{m+1} contributes *nothing* to the wanted eigenvectors and is wasted. It only indicates that residuals of $\lambda^{(m)}, \varphi^{(m)}$ are in its direction.

We want to exploit the available v_{m+1} and propose a new strategy that uses the Ritz values $\lambda^{(m)}$ obtained from $\mathcal{K}_m(v_1, A)$ but computes modified approximate eigenvectors $\psi^{(m)}$ in $\mathcal{K}_{m+1}(v_1, A)$. These new vectors are linear combinations of $\varphi^{(m)}$ and v_{m+1}, such that residual norm of each pair $\lambda^{(m)}, \psi^{(m)}$ is minimal over the span of $\varphi^{(m)}$ and v_{m+1}. They can be calculated by solving a two-dimensional minimization problem for each eigenvector. As a result, residual norms of the new approximate eigenpairs $\lambda^{(m)}, \psi^{(m)}$ are at least as small as those of $\lambda^{(m)}, \varphi^{(m)}$ and often dramatically smaller. The total extra cost of this strategy is one matrix-vector multiplication plus only $2r$ inner products, where r is the number of wanted eigenpairs and it is typically much smaller than m in practice. So the resulting modified m-step Arnoldi method is cheaper than the standard $(m+1)$-step one, which requires besides one matrix-vector multiplication at least $(m+1)$ inner products.

In Section 2 we review the m-step Arnoldi process and method as well as a few well-known properties for the motivation and use of our strategy; in Section 3 we describe the new strategy that chooses modified approximate eigenvectors in $\mathcal{K}_{m+1}(v_1, A)$. We establish a relationship between residual norms of the modified approximate eigenpairs and those of the Ritz pairs, and analyze it. We then present a modified m-step restarted Arnoldi algorithm, and report some numerical experiments in Section 4. They show that the modified m-step restarted algorithm and its version with Chebyshev acceleration are *often considerably more efficient* than the standard $(m+1)$-step restarted ones.

Some notation is introduced now. Assume A to be an $N \times N$ real matrix with eigenpairs λ_i, φ_i, where $\|\varphi_i\| = 1$, $i = 1, 2, \ldots, N$. Here the norm used is the Euclidean norm. We denote by the superscript $*$ the conjugate transpose of a matrix or vector and by the superscript $-$ the complex conjugate of a number. We are concerned with r eigenvalues λ with largest (smallest) real or largest imaginary parts and the corresponding eigenvectors φ, where $r \ll N$.

2 The m-step Arnoldi process and method

Given a real unit norm initial vector v_1, the m-step Arnoldi process generates an orthonormal basis $\{v_j\}_{j=1}^m$ of the Krylov subspace $\mathcal{K}_m(v_1, A)$ if $\dim(\mathcal{K}_m(v_1, A)) = m$. In this basis, the projected matrix of A onto $\mathcal{K}_m(v_1, A)$ is represented by an $m \times m$ upper Hessenberg matrix H_m with entries h_{ij}. The basis $\{v_j\}_{j=1}^m$ and the h_{ij} are computed as follows:

Algorithm 1. The m-step Arnoldi process

1. $v_1 = v_1/\|v_1\|$.
2. For $j = 1, 2, \ldots, m$ do
   2.1. $w = Av_j$;
   2.2. for $i = 1, 2, \ldots, j$ do
   $h_{ij} = v_i^* w$;
   $w = w - h_{ij} v_i$.
   2.3. $h_{j+1j} = \|w\|, v_{j+1} = w/h_{j+1j}$.

Algorithm 1 can be written in matrix form

$$AV_m = V_m H_m + h_{m+1m} v_{m+1} e_m^*, \tag{1}$$

where $V_m = (v_1, v_2, \ldots, v_m)$, and e_m is the mth coordinate vector of dimension m. It follows immediately from (1) that $H_m = V_m^* A V_m$ since $v_{m+1}^* V_m = 0$.

It is seen from Algorithm 1 or (1) that v_{m+1} is already available, so in fact we get an orthonormal basis of $\mathcal{K}_{m+1}(v_1, A)$ when the m-step Arnoldi process is performed. However, we only have H_m instead of H_{m+1} at hand at this time.

Let $\lambda_i^{(m)}, y_i^{(m)}$, $i = 1, 2, \ldots, m$ denote the eigenpairs of H_m with $\|y_i^{(m)}\| = 1$, and compute $\varphi_i^{(m)}, i = 1, 2, \ldots, m$ by

$$\varphi_i^{(m)} = V_m y_i^{(m)}. \tag{2}$$

Here $\lambda_i^{(m)}, \varphi_i^{(m)}$, $i = 1, 2, \ldots, m$ are called the Ritz values and Ritz vectors of A in $\mathcal{K}_m(v_1, A)$. The m-step Arnoldi method then uses m Ritz pairs $\lambda^{(m)}, \varphi^{(m)}$ to approximate m eigenpairs of A.

Obviously, v_{m+1} plays no role in calculating $\varphi^{(m)}$, so it contributes nothing to the wanted φ and is wasted.

From (1) and (2), we get

$$r_i^{(m)} := (A - \lambda_i^{(m)} I)\varphi_i^{(m)} = h_{m+1m} e_m^* y_i^{(m)} v_{m+1}. \tag{3}$$

Therefore, residuals $r_i^{(m)}$ are in the direction of v_{m+1}.

How good approximations are may be measured in terms of an a-posteriori bound

$$\|r_i^{(m)}\| = h_{m+1m} \mid e_m^* y_i^{(m)} \mid . \tag{4}$$

(4) can be used for a stopping criterion which cheaply checks sizes of the residuals without computing $\varphi_i^{(m)}$ explicitly by (2).

As was explained in the introduction, $\varphi_i^{(m)}$ may be bad approximations and even may not converge at all even if the corresponding $\lambda_i^{(m)}$ have converged. In the next section, we propose a modified strategy that exploits v_{m+1} for contributing information to the eigenvectors of A.

3 New strategy and a modified algorithm

3.1 New strategy

Rather than using $\varphi_i^{(m)}$ as approximate eigenvectors, we now choose unit norm vectors $\psi_i^{(m)} \in \mathcal{K}_{m+1}(v_1, A)$ of the form $\psi_i^{(m)} = \alpha_i \varphi_i^{(m)} + \beta_i v_{m+1}$ as *modified* approximate eigenvectors, $i = 1, 2, \ldots, m$, where each pair α_i, β_i is a solution to the minimization problem

$$\min_{|\alpha|^2+|\beta|^2=1} \|(A - \lambda_i^{(m)} I)(\alpha \varphi_i^{(m)} + \beta v_{m+1})\|. \tag{5}$$

Define the modified residuals $\hat{r}_i^{(m)}$ by

$$\hat{r}_i^{(m)} = (A - \lambda_i^{(m)} I)\psi_i^{(m)}. \tag{6}$$

Then $\|\hat{r}_i^{(m)}\|$ is at least as small as $\|r_i^{(m)}\|$, $i = 1, 2, \ldots, m$, so the modified pairs $\lambda_i^{(m)}, \psi_i^{(m)}$ are better than the Ritz pairs $\lambda_i^{(m)}, \varphi_i^{(m)}$.

Here note that the solution α_i, β_i for each i is unique up to a scaling of a complex number of unit length and depends on m, but we omit m without ambiguity. So we can take α_i to be real.

Let us define the vectors

$$z_i^{(m)} = \begin{pmatrix} \alpha_i y_i^{(m)} \\ \beta_i \end{pmatrix}. \tag{7}$$

Then

$$\psi_i^{(m)} = V_{m+1} z_i^{(m)}, \;\; i = 1, 2, \ldots, m \tag{8}$$

where $V_{m+1} = (v_1, v_2, \ldots, v_{m+1})$. Note that the resulting $\hat{r}_i^{(m)}$ are in $\mathcal{K}_{m+2}(v_1, A)$, but unlike $r_i^{(m+1)}$, they are not in the direction of v_{m+2}. α_i, β_i are calculated in Theorem 1.

Theorem 1 *Define the matrix* $B_{m,i} = \left(r_i^{(m)}, (A - \lambda_i^{(m)} I) v_{m+1} \right)$, *and the numbers* $\xi_i = \|(A - \lambda_i^{(m)} I) v_{m+1}\|^2$, $\eta_i = v_{m+1}^* (A - \lambda_i^{(m)} I) v_{m+1}$, $\gamma_i = \sqrt{\left(\|r_i^{(m)}\|^2 - \xi_i \right)^2 + 4\|r_i^{(m)}\|^2 \mid \eta_i \mid^2}$. *Then*

$$\|\hat{r}_i^{(m)}\| = \sigma_{\min}(B_{m,i}) = \sqrt{\frac{\|r_i^{(m)}\|^2 + \xi_i - \gamma_i}{2}}, \tag{9}$$

where $\sigma_{\min}(B_{m,i})$ *is the smallest singular value of* $B_{m,i}$, *and*

$$\alpha_i = \frac{\xi_i - \|r_i^{(m)}\|^2 + \gamma_i}{\sqrt{\left(\xi_i - \|r_i^{(m)}\|^2 + \gamma_i \right)^2 + 4\|r_i^{(m)}\|^2 \mid \eta_i \mid^2}}, \tag{10}$$

$$\beta_i = \frac{2 h_{m+1m} e_m^* y_i^{(m)} \bar{\eta}_i}{\|r_i^{(m)}\|^2 - \xi_i - \gamma_i} \alpha_i, \tag{11}$$

Proof. Recall that $r_i^{(m)} = (A - \lambda_i^{(m)} I) \varphi_i^{(m)}$. Then we have

$$\|\hat{r}_i^{(m)}\| = \min_{|\alpha|^2 + |\beta|^2 = 1} \left\| B_{m,i} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \right\| = \sigma_{\min}(B_{m,i}).$$

It can then be verified that (9)–(11) hold by carefully inspecting the eigenproblem of the 2×2 matrix $B_{m,i}^* B_{m,i}$. $\square$

Remarks.

1. From (4), (10) and (11), we have

$$\left| \frac{\beta_i}{\alpha_i} \right| = \frac{2\|r_i^{(m)}\| \mid \eta_i \mid}{\xi_i - \|r_i^{(m)}\|^2 + \gamma_i}. \tag{12}$$

It can be verified that $\left| \frac{\beta_i}{\alpha_i} \right|$ is increasing in $\|r_i^{(m)}\|$ for a fixed ξ_i and it is decreasing in ξ_i for a fixed $\|r_i^{(m)}\|$. Therefore, when either ξ_i is small or $\|r_i^{(m)}\|$ is large, $\left| \frac{\beta_i}{\alpha_i} \right|$

is relatively large. It means that in either case v_{m+1} makes more contributions to φ_i. Particularly, if $\|r_i^{(m)}\| = 0$, then $\mid \alpha_i \mid= 1$ and $\beta_i = 0$; if $\xi_i = 0$, then $\alpha_i = 0$ and $\mid \beta_i \mid= 1$ since in this case $\eta_i = 0$; if $\xi_i = \|r_i^{(m)}\|^2$, then $\mid \beta_i \mid=\mid \alpha_i \mid= \frac{1}{\sqrt{2}}$, which means that v_{m+1} and $\varphi_i^{(m)}$ make the same contribution to φ_i.

2. It can be derived from (9) that

$$\frac{\|\hat{r}_i^{(m)}\|}{\|r_i^{(m)}\|} \leq \frac{\|(I - v_{m+1}v_{m+1}^*)(A - \lambda_i^{(m)}I)v_{m+1}\|}{\|(A - \lambda_i^{(m)}I)v_{m+1}\|} < 1 \text{ if } \eta_i \neq 0. \tag{13}$$

It implies $\|\hat{r}_i^{(m)}\| = 0$ when the columns of $B_{m,i}$ are dependent no matter how $\|r_i^{(m)}\|$ is. $\psi_i^{(m)}$ is an exact eigenvector in this case. We may expect from (13) that the relative ratio $\|\hat{r}_i^{(m)}\|/\|r_i^{(m)}\|$ is small. This implies that $\|\hat{r}_i^{(m)}\|$ may be much smaller than $\|r_i^{(m)}\|$. As an effect, the modified $\psi_i^{(m)}$ may be much better than $\varphi_i^{(m)}$ when $\varphi_i^{(m)}$ is a bad approximation to φ_i and $\lambda_i^{(m)}$ is converging. From Theorem 1, we may consider β_i to be a controlling coefficient in some sense. As a remedy, v_{m+1} pulls $\varphi_i^{(m)}$ by adding a larger weight in the direction of v_{m+1} when $\lambda_i^{(m)}$ is converging but $\varphi_i^{(m)}$ is getting bad. Conversely, it will put a smaller weight on $\varphi_i^{(m)}$ if the pair $\lambda_i^{(m)}, \varphi_i^{(m)}$ is good.

3. Assume that $\lambda_i^{(m)}, \psi_i^{(m)}$ and $\lambda_i^{(m+1)}, \varphi_i^{(m+1)}$, $i = 1, 2, \ldots, r$ are used to approximate the r selected eigenpairs of A. Then although it is impossible to prove $\|\hat{r}_i^{(m)}\| \leq \|r_i^{(m+1)}\|$, $i = 1, 2, \ldots, r$, it is often the case in practice, particularly when $\lambda_i^{(m)}$ and $\lambda_i^{(m+1)}$ are good approximations but $\varphi_i^{(m)}$ and $\varphi_i^{(m+1)}$ are not.

3.2 A modified m-step restarted Arnoldi algorithm

After the above analysis, we can present the following algorithm.

Algorithm 2. The modified m-step restarted Arnoldi algorithm

1. Start: Given the number r of the wanted eigenpairs, choose the steps m of Arnoldi's process, a tolerance *tol* and an initial unit norm vector v_1.

2. Construct the upper Hessenberg matrix H_m and V_{m+1} by performing the m-step Arnoldi process.

3. Compute the eigenpairs $\lambda_i^{(m)}, y_i^{(m)}$, $i = 1, 2, \ldots, m$ of H_m. Then select r of the $\lambda_i^{(m)}$ as approximations to the r desired eigenvalues $\lambda_i, i = 1, 2, \ldots, r$.

4. If $h_{m+1m} \leq tol$, then all the $\|r_i^{(m)}\| \leq tol$. We then take Ritz vectors $\varphi_i^{(m)}$ as approximations to φ_i and stop, else take $\psi_i^{(m)}$ as approximations to φ_i and

calculate the residual norms of approximating $\lambda_i^{(m)}, \psi_i^{(m)}$, $i = 1, 2, \ldots, r$ by (9). If they are all below *tol*, then stop and compute $\psi_i^{(m)}$ by (8), else continue.

5. Construct a new initial unit norm vector v_1 from $\psi_i^{(m)}$, $i = 1, 2, \ldots, r$, and then return to Step 2.

For Step 2, in order to get an orthonormal basis numerically, as done in [11, 14], reorthogonalization is performed whenever severe cancellations occur. So, calculating v_{j+1} requires one matrix-vector multiplication and at least $(j+1)$ inner products.

For Step 5, we use a strategy adapted from Saad [11], where it is only necessary to replace the $y_i^{(m)}$ and Ritz vectors $\varphi_i^{(m)}$ by $z_i^{(m)}$ and $\psi_i^{(m)}$, $i = 1, 2, \ldots, r$, respectively.

The computation of $\psi_i^{(m)}, i = 1, 2, \ldots, r$ can be easily designed so that the total extra cost of the computations of $\|\hat{r}_i^{(m)}\|$ and α_i, β_i, $i = 1, 2, \ldots, r$ is one matrix-vector multiplication plus $2r$ inner products. So the modified m-step Arnoldi method is cheaper than the standard $(m+1)$-step one. Compared with the total cost of the standard m-step Arnoldi method, the latter requires not only one more matrix-vector multiplication and at least $(m+1)$ inner products but also the solution of the eigenproblem of a bigger H_{m+1}. If $r \ll m$ and inner products are relatively expensive in computations, the savings may be considerable at each restart. From a standpoint of the computational cost at each restart, to be fairer we should compare Algorithm 2 and its version with Chebyshev acceleration with the standard $(m+1)$-step restarted counterparts. Numerical experiments will show the superiority of the former ones.

4 Numerical experiments

We have tested Algorithm 2 and its version with Chebyshev acceleration, the standard restarted Arnoldi algorithm [11] and Arnoldi–Chebyshev algorithm [3, 13] using MATLAB4.2 on a DEC RISC workstation with the machine precision $eps \approx 2.22 \times 10^{-16}$. The efficiency of these algorithms can thus be measured in terms of the number of restarts (iterations) *it* or matrix-vector multiplications *m.v.*

Example 1. This is a common test problem; see, e.g., [11, 14]. Consider the convection diffusion differential equation

$$-\triangle u(x, y) + \rho u_x = \lambda u(x, y)$$

on a square region $[0, 1] \times [0, 1]$ with the boundary condition $u(x, y) = 0$.

Taking $\rho = 1$ and discretizing with centered differences yield the block tridiagonal matrix $A(n) = \mathrm{tri}(-I, B_n, -I)$, where $B_n = \mathrm{tri}(b, 4, a)$, n is chosen the number of interior mesh points on each side of the square, and $a = -1 + 1/2(n+1)$, $b = -1 - 1/2(n+1)$.

Algorithm 2 and the standard restarted Arnoldi algorithm were run on the 576×576 matrix $A(24)$ obtained by taking $n = 24$. We compute the three eigenvalues with largest real parts and the associated eigenvectors. We require that both algorithms be stopped as soon as all the residual norms of $\lambda_i^{(m)}, \varphi_i^{(m)}$ and $\lambda_i^{(m)}, \psi_i^{(m)}$, $i = 1, 2, 3$ are below $tol = 10^{-8}$. Both algorithms used the same initial vector v_1 generated randomly in a normal distribution. Table 1 shows the results obtained for different m.

Table 1: *Example 1,* $\lambda_1 \approx 7.96806192, \lambda_2 \approx 7.92100825, \lambda_3 \approx 7.92099884$. *Left: the standard restarted Arnoldi algorithm; Right: Algorithm 2.*

m	it	$m.v$	Max.Res.Norms	m	it	$m.v$	Max.Res.Norms
66	102	6732	$2.7E-9$	65	26	1716	$8.6E-9$
71	18	1278	$4.9E-9$	70	13	923	$5.5E-9$
76	11	836	$5.6E-9$	75	6	456	$5.E-10$
81	6	486	$5.5E-10$	80	4	324	$1.7E-9$

It is seen from Table 1 that Algorithm 2 with steps m was considerably more efficient than the standard $(m+1)$-step restarted Arnoldi algorithm, as shown by it or $m.v$. This shows that v_{m+1}, at least at some restarts, indeed made essential contributions to the wanted eigenvectors and thus greatly improved the overall performance of the standard algorithm. Figures 1–2 depict the convergence curves of the standard restarted Arnoldi algorithm with $m = 66$ and Algorithm 2 with $m = 65$, respectively. They show that the standard restarted Arnoldi algorithm exhibited very irregular convergence behavior, while, in contrast, Algorithm 2 converged much more smoothly. The irregular convergence behavior may be explained by the theoretical analysis in [4, 7, 8]. So, to some extent, our strategy has the effect of smoothing possible irregular behavior of the standard algorithm.

As a by-product, we now report some results obtained by Algorithm 2 with Chebyshev acceleration and the standard restarted Arnoldi–Chebyshev algorithm for various m and n_c, where n_c is the steps of Chebyshev acceleration. In the experiments, we used the same v_1 in the modified and standard restarted Arnoldi–Chebyshev algorithms, and the stopping requirement and the notation used were as before. Table 2 lists the results.

We can see from Table 2 that the Chebyshev acceleration had a remarkable effect on both the standard and modified restarted Arnoldi–Chebyshev algorithms. As a result, the number of restarts has been reduced considerably. However, the modified m-step restarted Arnoldi–Chebyshev algorithm was often considerably more efficient than the standard $(m+1)$-step restarted Arnoldi–Chebyshev algorithm. But we should mention that the use of Chebyshev iteration has some limitations. For example, firstly, it can only be used to compute the right-most or left-most eigenpairs; secondly, for many

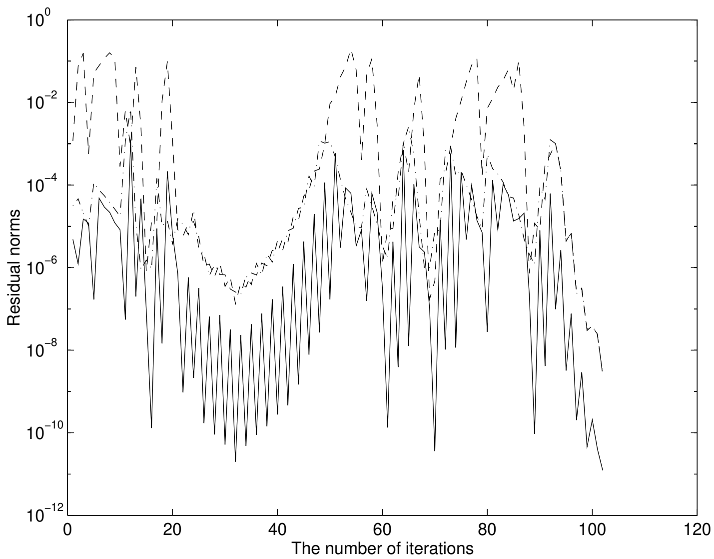

Figure 1: *Example 1, the standard restarted Arnoldi algorithm with* $m = 66$*. Solid line: error of* $\lambda_1^{(m)}, \varphi_1^{(m)}$*, dashdot line: error of* $\lambda_2^{(m)}, \varphi_2^{(m)}$ *and dash line: error of* $\lambda_3^{(m)}, \varphi_3^{(m)}$*.*

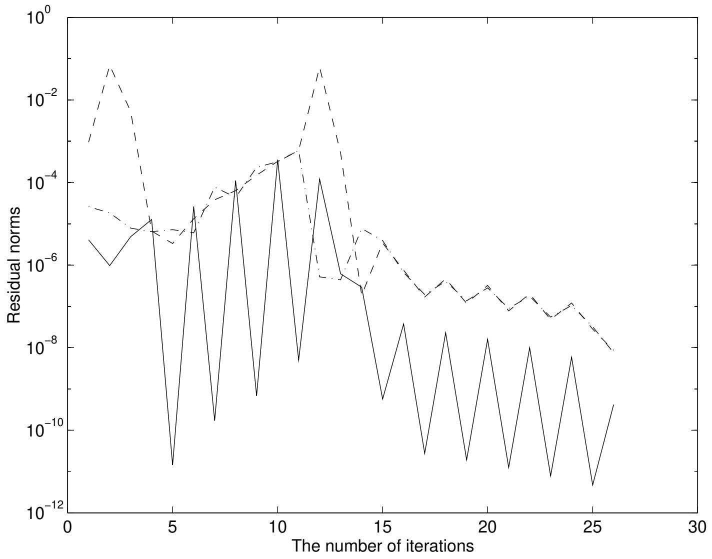

Figure 2: *Example 1, Algorithm 2 with* $m = 65$*. Solid line: error of* $\lambda_1^{(m)}, \psi_1^{(m)}$*, dashdot line: error of* $\lambda_2^{(m)}, \psi_2^{(m)}$ *and dash line: error of* $\lambda_3^{(m)}, \psi_3^{(m)}$*.*

Table 2: *Example 1, Left: the standard restarted Arnoldi–Chebyshev algorithm; Right: Algorithm 2 with Chebyshev acceleration.*

m	n_c	it	$m.v$	Max.Res.Norms	m	n_c	it	$m.v$	Max.Res.Norms
31	40	29	2019	$3.2E-11$	30	40	23	1593	$8.4E-10$
31	50	15	1165	$3.2E-12$	30	50	10	760	$3.5E-10$
31	60	6	486	$8.7E-11$	30	60	5	395	$9.4E-10$
41	40	9	689	$9.E-11$	40	40	6	440	$6.4E-9$
41	50	8	678	$7.5E-10$	40	50	5	405	$3.3E-9$
41	60	5	445	$5.9E-10$	40	60	4	344	$7.8E-9$
51	40	8	688	$2.9E-10$	50	40	6	506	$9.4E-10$
51	50	6	556	$1.2E-9$	50	50	5	455	$4.5E-9$
51	60	5	495	$1.1E-11$	50	60	4	435	$3.7E-11$

non-normal matrices, it could gain little, e.g., [9]; thirdly, a robust and efficient choice of n_c is often difficult.

Example 2. This example is the Tolosa matrix from aerodynamics related to the stability analysis of a model of a plane in flight [2]. The interesting modes of this system are described by complex eigenvalues whose imaginary parts lie in a frequency range chosen by engineers. We are interested in a few eigenvalues with largest imaginary parts and the associated eigenvectors. The matrix A here is sparse and highly non-normal, and has order N greater than or equal to 90 and N is always a multiple of 5. Since the eigenproblem of A is very ill conditioned, it can be very difficult to compute a few eigenpairs of it. In the following experiments, we compute the three eigenvalues with largest imaginary parts for $N = 500, 800$. We require that Algorithm 2 and the restarted Arnoldi algorithm be stopped as soon as residual norms of $\lambda_i^{(m)}, \varphi_i^{(m)}$ and $\lambda_i^{(m)}, \psi_i^{(m)}$, $i = 1, 2, 3$ are below $tol = 10^{-6}$. Since the wanted eigenvalues are complex, we in fact get six eigenpairs as A is real. Tables 3–4 give the results obtained.

It can be seen from Tables 3–4 that Algorithm 2 with steps m had great improvements on the standard $(m+1)$-step restarted Arnoldi algorithm in most cases, as shown by it or $m.v$. This again shows that v_{m+1}, at least at some restarts, made significant contributions to the wanted eigenvectors. As in Example 1, Algorithm 2 converged considerably more smoothly than the restarted Arnoldi algorithm did. Only for quite large m, the standard $(m+1)$ restarted Arnoldi algorithm was nearly as efficient as the modified m-step restarted Arnoldi algorithm. Also, the standard restarted Arnoldi algorithm with a larger m does not necessarily result in fewer restarts than that with a smaller m, as is seen from the tables. This is not surprising both in theory and numerical computations; for a detailed analysis, see [4, 7, 8]. Figures 3–4 describe the

Table 3: *Tolosa matrix of* $N = 500$, $\|AA^* - A^*A\|_F \approx 8.46E+11, \|AA^* - A^*A\|_F/\|A\|_F \approx 4.39E+5$. $\lambda_1 \approx -190.25905 + 613.16025i, \lambda_2 \approx -186.16185 + 608.14453i, \lambda_3 \approx -182.10841 + 603.10573i$. *Left: the standard restarted Arnoldi algorithm; Right: Algorithm 2.*

m	it	$m.v$	Max.Res.Norms	m	it	$m.v$	Max.Res.Norms
46	42	1932	$7.3E-7$	45	24	1104	$6.6E-7$
51	60	3060	$6.2E-7$	50	17	867	$1.2E-7$
56	21	1176	$5.3E-7$	55	9	504	$8.2E-7$
61	20	1220	$1.4E-7$	60	6	366	$1.1E-7$
66	5	330	$1.1E-7$	65	4	264	$3.4E-7$
71	9	639	$7.2E-9$	70	3	213	$3.9E-8$

Table 4: *Tolosa matrix of* $N = 800$, $\|AA^* - A^*A\|_F \approx 6.22E+12, \|AA^* - A^*A\|_F/\|A\|_F \approx 1.06E+6$. $\lambda_1 \approx -298.49015 + 956.50804i, \lambda_2 \approx -294.60558 + 951.43237i, \lambda_3 \approx -290.74627 + 946.34381i$. *Left: the standard restarted Arnoldi algorithm; Right: Algorithm 2.*

m	it	$m.v$	Max.Res.Norms	m	it	$m.v$	Max.Res.Norms
56	238	13328	$3.3E-7$	55	29	1479	$8.9E-7$
61	100	6100	$7.7E-8$	60	21	1281	$3.9E-7$
66	27	1782	$3.E-7$	65	12	792	$1.9E-7$
71	28	1988	$4.5E-8$	70	11	781	$2.1E-8$
76	17	1292	$6.6E-7$	75	9	684	$1.6E-8$
81	7	567	$6.7E-7$	80	6	486	$1.6E-9$

convergence processes of the standard restarted Arnoldi algorithm with $m = 61$ and Algorithm 2 with $m = 60$ when $N = 800$.

A number of other matrices, e.g., the Clement matrix from the set of test matrices in the *netlib* and a class of random walk matrices in Markov chains [11], have been tested, showing that the modified m-step restarted algorithms often exhibit a remarkable superiority to the standard $(m+1)$-step restarted ones.

5 Concluding remarks

The standard restarted Arnoldi algorithm and its variants may not be efficient for computing a few selected eigenpairs of large unsymmetric matrices. In order to improve the overall performance of Arnoldi type algorithms, we have proposed the modified strategy that uses the Ritz values obtained from $\mathcal{K}_m(v_1, A)$ but chooses modified approximate eigenvectors in $\mathcal{K}_{m+1}(v_1, A)$, such that each modified residual is minimal over the span of the Ritz vector and the $(m+1)$th basis vector. The numerical ex-

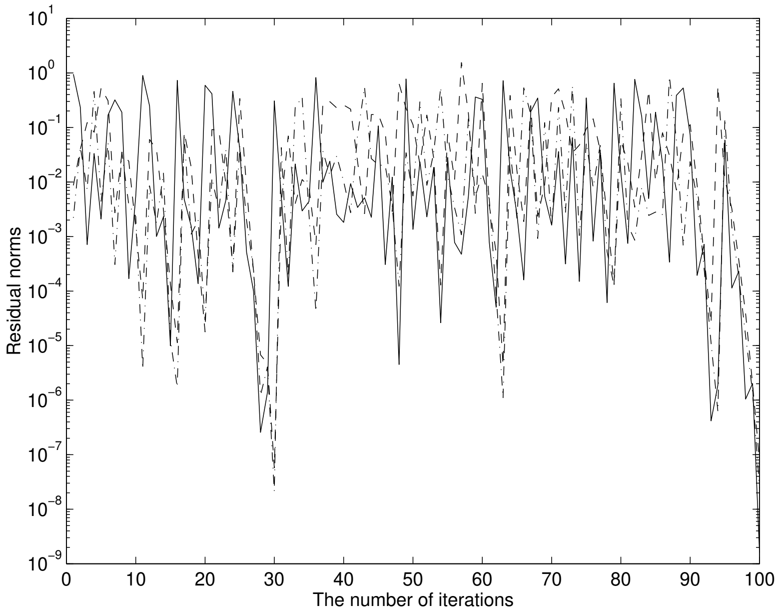

Figure 3: *Tolosa matrix of* $N = 800$*, the standard restarted Arnoldi algorithm with* $m = 61$*. Solid line: error of* $\lambda_1^{(m)}, \varphi_1^{(m)}$*, dashdot line: error of* $\lambda_2^{(m)}, \varphi_2^{(m)}$ *and dash line: error of* $\lambda_3^{(m)}, \varphi_3^{(m)}$*.*

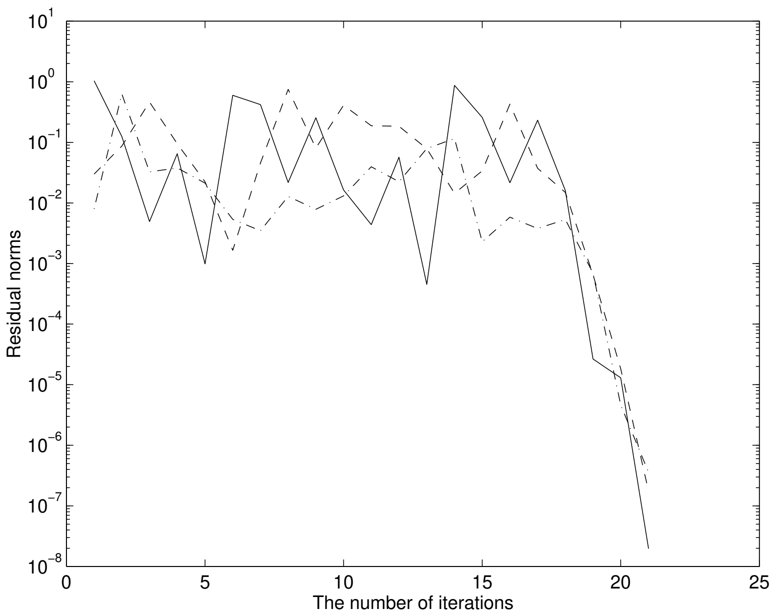

Figure 4: *Tolosa matrix of* $N = 800$*, Algorithm 2 with* $m = 60$*. Solid line: error of* $\lambda_1^{(m)}, \psi_1^{(m)}$*, dashdot line: error of* $\lambda_2^{(m)}, \psi_2^{(m)}$ *and dash line: error of* $\lambda_3^{(m)}, \psi_3^{(m)}$*.*

periments have demonstrated that the modified m-step restarted algorithms are often much more efficient than the standard $(m+1)$-step restarted ones.

We point out that the strategy presented in the paper can be applied to other variants of Arnoldi's method as well. A similar strategy could be extended to the block Arnoldi method [5]. Also, this strategy may be used in some Krylov subspace type methods for the solution of large unsymmetric linear systems, e.g., Arnoldi's method or FOM and the GMRES method, where the available $(m+1)$th basis vector can be used to improve the quality of an approximate solution in $\mathcal{K}_m(v_1, A)$. In a proper way, a modified approximate solution will lie in $\mathcal{K}_{m+1}(v_1, A)$ and have a smaller residual norm than that of the original one.

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