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A Refined Shift-and-Invert Arnoldi Algorithm for Large Unsymmetric Generalized Eigenproblems

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Abstract—The shift-and-invert Arnoldi method has been popularly used for computing a number of eigenvalues close to a given shift and/or the associated eigenvectors of a large unsymmetric matrix pair, but there is no guarantee for the approximate eigenvectors, Ritz vectors, obtained by this method to converge even though the subspace is good enough. In order to correct this problem, a refined shift-and-invert Arnoldi method is proposed that uses certain refined Ritz vectors to approximate the desired eigenvectors. The refined Ritz vectors can be computed cheaply and reliably by small-sized singular value decompositions. It is shown that the refined method converges. A refined shift-and-invert Arnoldi algorithm is developed, and several numerical examples are reported. Comparisons are drawn on the refined algorithm and the shift-and-invert Arnoldi algorithm, indicating that the former is considerably more efficient than the latter.

Keywords—Large generalized eigenproblem, Matrix pair, Shift-and-invert, Arnoldi method, Refined Arnoldi method, Ritz value, Ritz vector, Refined Ritz vector, Convergence.

1. INTRODUCTION

Consider the large unsymmetric generalized eigenproblem

$$A\varphi_i = \lambda_i B\varphi_i, \tag{1}$$

where A and B are $N \times N$ large matrices. In many scientific applications, e.g., [1], we are interested in computing some interior eigenvalues of A in the complex plane, i.e., some eigenvalues close to a given shift σ and/or the associated eigenvectors of the above matrix pair (A, B). The problem is so large that it cannot be treated by standard numerical methods for small- and medium-sized

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matrices, but it is supposed that an LU factorization of a nonsingular matrix $A - \sigma B$ is feasible and can be done at reasonable cost.

One of the most commonly used techniques for this kind of problem is the shift-and-invert Arnoldi method [2], which is a natural generalization of the shift-and-invert Lanczos method for the symmetric case [3,4]. When $A - \sigma B$ is invertible for σ, the eigenvectors of the matrix pair (A, B) are the same as those of the matrix $(A - \sigma B)^{-1}B$. Therefore, we can run the Arnoldi method on the matrix $(A - \sigma B)^{-1}B$. The eigenvalues of (A, B) can also be recovered from the computed eigenvalues.

If the shift σ is suitably selected, the distribution of the spectrum of the transformed matrix $C = (A - \sigma B)^{-1}B$ may be favorable even if the eigenvalues close to the shift σ of the matrix pair (A, B) are clustered. Therefore, the Arnoldi method applied to the eigenproblem of the shift-and-invert matrix C may give a much faster convergence with eigenvalues close to the shift σ. Furthermore, instead of a fixed or constant shift σ, Ruhe provided an effective technique [5–9] on selecting the shifts σ dynamically so that the resulting variant, called rational Krylov algorithms, may be more efficient.

However, it has been shown that the Arnoldi method may not converge [10–12]: the approximate eigenvectors, Ritz vectors, obtained by this method may converge erratically and even may not converge though the Krylov subspace contains sufficient information on the desired eigenvectors and the corresponding approximate eigenvalues, Ritz values, converge. In fact, such a possible nonconvergence may occur to general standard projection methods, as shown in [11,12]. To correct this problem, Jia has proposed a class of refined projection methods that have a mathematically different background from the standard methods for extracting eigenvectors. Several refined algorithms have been developed, and they have shown their (far) superiority to their corresponding standard counterparts [13–18]. Stewart [19] and van der Vorst [20] have given an excellent and quite detailed account of the refined methods.

Since the shift-and-invert Arnoldi method for problem (1) is mathematically equivalent to the Arnoldi method for solving the transformed eigenproblem, the former has the same convergence problem as the latter does. This motivates us to derive a refined shift-and-invert Arnoldi method and to develop corresponding more efficient algorithms. The refined method uses refined Ritz vectors with minimal residuals to approximate the desired eigenvectors of the matrix pair (A, B). The refined Ritz vectors can be obtained by some small-sized singular value decompositions (SVD). It is shown that the refined method converges under a natural hypothesis that a Krylov subspace is good enough. Based on the MATLAB function `sptarn.m` due to Ruhe [21], we make a modification to it and develop a refined shift-and-invert Arnoldi algorithm. We then report several numerical examples and compare the refined algorithm with the shift-and-invert Arnoldi algorithm. Numerical experiments show that the former is considerably more efficient than the latter.

The paper is organized as follows. Section 2 describes the shift-and-invert Arnoldi method and some properties of it. Section 3 proposes the refined shift-and-invert Arnoldi method and establishes some results on it, and it then presents a refined shift-and-invert Arnoldi algorithm. Section 4 considers the convergence of the refined shift-and-invert Arnoldi method. Section 5 discusses implementational details. Finally, Section 6 reports numerical results on four real world problems and draws comparisons on the two algorithms.

Throughout this paper, assume that the matrix pair (A, B) is regular; i.e., there exists a shift σ such that the matrix $A - \sigma B$ is not singular. Let $C = (A - \sigma B)^{-1}B$, and denote by C^m the vector space of dimension m. For a unit norm vector v_1, let $\mathcal{K}_m(C, v_1)$ denote the Krylov subspace spanned by $v_1, Cv_1, \ldots, C^{m-1}v_1$ and π_m the orthogonal projector onto $\mathcal{K}_m(C, v_1)$. The norm used in this paper is the Euclidean norm. We denote by an asterisk the conjugate transpose of a matrix or vector and by $\sigma_{\min}(X)$ the smallest singular values of a matrix. Let I_m be the $m \times m$ identity matrix and $\tilde{I}_m$ the $(m+1) \times m$ matrix which is the same as I_m with an additional zero row.

2. THE SHIFT-AND-INVERT ARNOLDI METHOD

If the matrix $A - \sigma B$ is invertible for some shift σ, the eigenproblem (1) can be transformed into the standard eigenproblem

$$C\varphi_i = \theta_i \varphi_i, \tag{2}$$

where $\theta_i = 1/(\lambda_i - \sigma)$.

It is easy to verify that (λ_i, φ_i) is an eigenpair of problem (1) if and only if (θ_i, φ_i) is an eigenpair of the matrix C. Therefore, the shift-and-invert Arnoldi method for the eigenproblem (1) is mathematically equivalent to the standard Arnoldi method for the transformed eigenproblem (2). It starts with a given unit length vector v_1 (usually chosen randomly) and builds up an orthonormal basis V_m for the Krylov subspace $\mathcal{K}_m(C, v_1)$ by means of the Gram-Schmidt orthogonalization process. In finite precision, reorthogonalization is performed whenever some severe cancellation occurs [2]. Then the approximate eigenpairs for the transformed eigenproblem (2) can be extracted from $\mathcal{K}_m(C, v_1)$. The approximate solutions for problem (1) can be recovered from these approximate eigenpairs.

The shift-and-invert Arnoldi process can be written in matrix form

$$(A - \sigma B)^{-1} B V_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^* \tag{3}$$

or

$$(A - \sigma B)^{-1} B V_m = V_{m+1} \tilde{H}_m, \tag{4}$$

where e_m is the m^{th} coordinate vector of dimension m, $V_{m+1} = (V_m, v_{m+1}) = (v_1, v_2, \ldots, v_{m+1})$ is an $N \times (m+1)$ matrix whose columns form an orthonormal basis of the $(m+1)$-dimensional Krylov subspace $\mathcal{K}_{m+1}(C, v_1)$, and $\tilde{H}_m$ is the $(m+1) \times m$ upper Hessenberg matrix that is the same as H_m except for an additional row whose only nonzero entry is $h_{m+1,m}$ in the position $(m+1, m)$.

Suppose that $(\tilde{\theta}_i, \tilde{y}_i)$, $i = 1, 2, \ldots, m$ are the eigenpairs of the matrix H_m,

$$H_m \tilde{y}_i = \tilde{\theta}_i \tilde{y}_i. \tag{5}$$

Let

$$\tilde{\lambda}_i = \sigma + \frac{1}{\tilde{\theta}_i} \qquad \text{and} \qquad \tilde{\varphi}_i = V_m \tilde{y}_i. \tag{6}$$

Then the shift-and-invert Arnoldi method uses $(\tilde{\lambda}_i, \tilde{\varphi}_i)$ to approximate the eigenpairs (λ_i, φ_i) of problem (1). The $\tilde{\lambda}_i$ and $\tilde{\varphi}_i$ are called the Ritz values and the Ritz vectors of A with respect to $\mathcal{K}_m(C, v_1)$, respectively. Define the corresponding residual

$$\tilde{r}_i = \left(A - \tilde{\lambda}_i B\right) \tilde{\varphi}_i. \tag{7}$$

Then we have the following theorem.

THEOREM 2.1. *The residuals $\tilde{r}_i$ corresponding to the approximate eigenpairs $(\tilde{\lambda}_i, \tilde{\varphi}_i)$ by the shift-and-invert Arnoldi method satisfy*

$$\|\tilde{r}_i\| \le h_{m+1,m} \left|\tilde{\lambda}_i - \sigma\right| \|A - \sigma B\| \left|e_m^* \tilde{y}_i\right|. \tag{8}$$

PROOF. From relations (3), (4), and (6), we obtain

$$\begin{aligned}
\|\tilde{r}_i\| &= \left\|\left(A-\tilde{\lambda}_i B\right)\tilde{\varphi}_i\right\| \\
&= \left\|\left(A-\tilde{\lambda}_i B\right)V_m\tilde{y}_i\right\| \\
&= \left\|\left((A-\sigma B)-\left(\tilde{\lambda}_i-\sigma\right)B\right)V_m\tilde{y}_i\right\| \\
&= \left\|(A-\sigma B)\left(I-\left(\tilde{\lambda}_i-\sigma\right)(A-\sigma B)^{-1}B\right)V_m\tilde{y}_i\right\| \\
&= \left|\tilde{\lambda}_i-\sigma\right|\left\|(A-\sigma B)\left((A-\sigma B)^{-1}B-\tilde{\theta}_i I\right)V_m\tilde{y}_i\right\| \\
&\le \left|\tilde{\lambda}_i-\sigma\right|\|A-\sigma B\|\left\|V_{m+1}\left(\tilde{H}_m-\tilde{\theta}_i\tilde{I}_m\right)\tilde{y}_i\right\| \\
&= h_{m+1,m}\left|\tilde{\lambda}_i-\sigma\right|\|A-\sigma B\|\left|e_m^*\tilde{y}_i\right|.
\end{aligned}$$

∎

Ruhe has developed a shift-and-invert Arnoldi algorithm; see, e.g., `sptarn.m` in MATLAB where it is designed to compute all the eigenvalues in a rectangle and the associated eigenvectors. The algorithm can be modified to compute the k eigenvalues near a target point σ and the associated eigenvectors. We call the resulting algorithm Algorithm 1. For details, refer to Section 5.

3. A REFINED SHIFT-AND-INVERT ARNOLDI METHOD

To correct the possible nonconvergence of Ritz vectors, Jia has proposed a class of refined projection methods [11,13,16] for the standard eigenproblem: for each approximate eigenvalue available, say, Ritz value, seek a unit length refined Ritz vector from the subspace to approximate the wanted eigenvector. The refined Ritz vector minimizes the corresponding residual norm formed with the approximate eigenvalue over the subspace. This implies that the refined Ritz vector is the best approximation to the wanted eigenvector over the subspace with respect to the Euclidean norm and the approximate eigenvalue.

The principle of the refined methods can be applied to the shift-and-invert Arnoldi method for the generalized eigenproblem in the following way. For each $\tilde{\theta}_i$, seek a unit length vector $u_i \in \mathcal{K}_m(C, v_1)$ that satisfies the following optimality property:

$$\left\|\left((A-\sigma B)^{-1}B-\tilde{\theta}_i I\right)u_i\right\| = \min_{\substack{u\in\mathcal{K}_m(C,v_1)\\ \|u\|=1}}\left\|\left((A-\sigma B)^{-1}B-\tilde{\theta}_i I\right)u\right\|. \tag{9}$$

We use $(\tilde{\lambda}_i, u_i)$ to approximate the eigenpair (λ_i, φ_i) of (A, B). So u_i is the best approximation to φ_i from $\mathcal{K}_m(C, v_1)$ with respect to $\tilde{\theta}_i$ and the Euclidean norm, and thus is called a refined Ritz vector. The resulting method is referred to as the refined shift-and-invert Arnoldi method. Clearly, the mathematical background for the refined method is now different from that of the original method.

Denote the residual norm of the refined approximate eigenpair $(\tilde{\lambda}_i, u_i)$ by

$$\|\hat{r}_i\| = \left\|\left(A-\tilde{\lambda}_i B\right)u_i\right\|. \tag{10}$$

Then we have the following result.

THEOREM 3.1. *Assume z_i to be the right singular vector associated with the smallest singular value $\sigma_{\min}(\tilde{H}_m-\tilde{\theta}_i\tilde{I}_m)$ of the $(m+1)\times m$ Hessenberg matrix $\tilde{H}_m-\tilde{\theta}_i\tilde{I}_m$. Then*

$$u_i = V_m z_i, \tag{11}$$

$$\|\hat{r}_i\| \le \left|\tilde{\lambda}_i-\sigma\right|\|A-\sigma B\|\sigma_{\min}\left(\tilde{H}_m-\tilde{\theta}_i\tilde{I}_m\right). \tag{12}$$

If the shift-and-invert Arnoldi process breaks down, i.e., $h_{m+1,m} = 0$, then $u_i = \tilde{\varphi}_i = \varphi_i$ and $\tilde{\lambda}_i = \lambda_i$, $i = 1, 2, \ldots, m$.

PROOF. Since V_m and V_{m+1} are orthonormal, we have from (4), (9), and (10) that

$$\begin{aligned}
\left\|\left((A-\sigma B)^{-1}B - \tilde{\theta}_i I\right) u_i\right\| &= \min_{\substack{z\in C^m \\ \|z\|=1}} \left\|\left((A-\sigma B)^{-1}B - \tilde{\theta}_i I\right) V_m z\right\| \\
&= \min_{\substack{z\in C^m \\ \|z\|=1}} \left\|V_{m+1}\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right) z\right\| \\
&= \min_{\substack{z\in C^m \\ \|z\|=1}} \left\|\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right) z\right\| \\
&= \left\|\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right) z_i\right\| \\
&= \sigma_{\min}\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right)
\end{aligned}$$

and

$$\begin{aligned}
\|\hat{r}_i\| &= \left\|\left(A - \tilde{\lambda}_i B\right) V_m z_i\right\| \\
&= \left\|\left((A-\sigma B) - \left(\tilde{\lambda}_i - \sigma\right) B\right) V_m z_i\right\| \\
&= \left\|(A-\sigma B)\left(I - \left(\tilde{\lambda}_i - \sigma\right)(A-\sigma B)^{-1}B\right) V_m z_i\right\| \\
&= \left|\tilde{\lambda}_i - \sigma\right| \left\|(A-\sigma B)\left((A-\sigma B)^{-1}B - \tilde{\theta}_i I\right) V_m z_i\right\| \\
&\le \left|\tilde{\lambda}_i - \sigma\right| \|A-\sigma B\| \left\|V_{m+1}\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right) z_i\right\| \\
&= \left|\tilde{\lambda}_i - \sigma\right| \|A-\sigma B\| \left\|\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right) z_i\right\| \\
&= \left|\tilde{\lambda}_i - \sigma\right| \|A-\sigma B\| \sigma_{\min}\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right).
\end{aligned}$$

Moreover, if $h_{m+1,m} = 0$, we get from Theorem 2.1

$$\left\|\left(A - \tilde{\lambda}_i B\right) \tilde{\varphi}_i\right\| = 0, \qquad i = 1, 2, \ldots, m. \tag{13}$$

Thus, $\tilde{\lambda}_i = \lambda_i$ and $\tilde{\varphi}_i = \varphi_i$, $i = 1, 2, \ldots, m$. ∎

From the above discussion, we can present the following algorithm.

ALGORITHM 2. A REFINED SHIFT-AND-INVERT ARNOLDI ALGORITHM (RSIA).

1. *Start*: Given m, the dimension of the Krylov subspace, k, the number of desired eigenpairs, and a tolerance tol. Choose an initial unit length vector v_1 and shift σ.
2. *Iterate*: For $j = 1, 2, \ldots, m$, do
   (a) Compute $r := (A-\sigma B)^{-1}Bv_j$.
   (b) Orthogonalize $r := r - V_j h_j$ where $h_j = V_j^* r$ (Gram-Schmidt).
   (c) Get new vector $v_{j+1} = r/h_{j+1,j}$, where $h_{j+1,j} = \|r\|$ (normalize).
3. *Approximate solutions*: Compute the approximate solutions $\tilde{\lambda}_i$ and u_i by relations (9)–(11) and use the pairs $(\tilde{\lambda}_i, u_i)$ to approximate the eigenpairs (λ_i, φ_i) of (A, B), $i = 1, 2, \ldots, k$.
4. *Test for convergence*: If all the residual norms $\|\hat{r}_i\|$, $i = 1, 2, \ldots, k$, are below tol, then stop, else continue.
5. *Restart*: Construct a new initial unit length vector v_1 and go to Step 2.

4. THE CONVERGENCE OF THE REFINED SHIFT-AND-INVERT ARNOLDI METHOD

The following result shows that the refined shift-and-invert Arnoldi method indeed converges under a natural hypothesis that the deviation of a required eigenvector from the subspace tends to zero.

THEOREM 4.1. *Define* $\xi = \|A - \sigma B\|\|(A - \sigma B)^{-1}B\|$ *and assume that* $\varepsilon = \|(I - \pi_m)\varphi_i\| \to 0$, *where* π_m *is the orthogonal projector on* $\mathcal{K}_m(C, v_1)$. *Then the approximate eigenpair* $(\tilde{\lambda}_i, u_i)$ *satisfies*

$$\left\|\left(A - \tilde{\lambda}_i B\right) u_i\right\| \le \xi \left|\tilde{\lambda}_i - \sigma\right| \frac{2\varepsilon + \left(2 + \varepsilon/\sqrt{1-\varepsilon^2}\right)\left(\varepsilon/\sqrt{1-\varepsilon^2}\right)^{1/m}}{\sqrt{1-\varepsilon^2}}. \tag{14}$$

If $\tilde{\theta}_i$ *is simple, then*

$$\left\|\left(A - \tilde{\lambda}_i B\right) u_i\right\| \le \xi \left|\tilde{\lambda}_i - \sigma\right| \frac{(2 + s_i)\varepsilon}{\sqrt{1-\varepsilon^2}} + O\left(\varepsilon^2\right), \tag{15}$$

where s_i *is the spectral condition number of* $\tilde{\theta}_i$.

PROOF. The eigenvalue $\tilde{\theta}_i$ of the matrix H_m satisfies

$$\begin{aligned}\left|\tilde{\theta}_i\right| \le \|H_m\| &= \left\|V_m^*(A - \sigma B)^{-1}BV_m\right\| \\ &\le \left\|(A - \sigma B)^{-1}B\right\|.\end{aligned}$$

From a result of [12], we have

$$\begin{aligned}\left|\theta_i - \tilde{\theta}_i\right| &\le \left\|(A - \sigma B)^{-1}B\right\| \left(2 + \frac{\varepsilon}{\sqrt{1-\varepsilon^2}}\right)^{1-1/m} \left(\frac{\varepsilon}{\sqrt{1-\varepsilon^2}}\right)^{1/m} \\ &\le \left\|(A - \sigma B)^{-1}B\right\| \left(2 + \frac{\varepsilon}{\sqrt{1-\varepsilon^2}}\right) \left(\frac{\varepsilon}{\sqrt{1-\varepsilon^2}}\right)^{1/m}.\end{aligned}$$

Therefore, we get from Theorem 7.1 that

$$\begin{aligned}\left\|\left(A - \tilde{\lambda}_i B\right) u_i\right\| &= \left\|\left((A - \sigma B) - \left(\tilde{\lambda}_i - \sigma\right) B\right) u_i\right\| \\ &= \left\|(A - \sigma B)\left(I - \left(\tilde{\lambda}_i - \sigma\right)(A - \sigma B)^{-1}B\right) u_i\right\| \\ &\le \left|\tilde{\lambda}_i - \sigma\right| \|A - \sigma B\| \left\|\left((A - \sigma B)^{-1}B - \tilde{\theta}_i I\right) u_i\right\| \\ &\le \left|\tilde{\lambda}_i - \sigma\right| \|A - \sigma B\| \min_{\substack{u \in \mathcal{K}_m(C, v_1) \\ \|u\| = 1}} \left\|\left((A - \sigma B)^{-1}B - \tilde{\theta}_i I\right) u\right\| \\ &\le \left|\tilde{\lambda}_i - \sigma\right| \|A - \sigma B\| \frac{\left\|(A - \sigma B)^{-1}B - \tilde{\theta}_i I\right\| \varepsilon + \left|\theta_i - \tilde{\theta}_i\right|}{\sqrt{1-\varepsilon^2}} \\ &\le \left|\tilde{\lambda}_i - \sigma\right| \|A - \sigma B\| \frac{\left(\left\|(A - \sigma B)^{-1}B\right\| + \left|\tilde{\theta}_i\right|\right) \varepsilon + \left|\theta_i - \tilde{\theta}_i\right|}{\sqrt{1-\varepsilon^2}} \\ &\le \xi \left|\tilde{\lambda}_i - \sigma\right| \frac{2\varepsilon + \left(2 + \varepsilon/\sqrt{1-\varepsilon^2}\right)\left(\varepsilon/\sqrt{1-\varepsilon^2}\right)^{1/m}}{\sqrt{1-\varepsilon^2}}.\end{aligned}$$

If $\tilde{\theta}_i$ is simple, then according to Theorem 3.7 of [10], we have

$$\left|\theta_i - \tilde{\theta}_i\right| \le s_i \left\|(A - \sigma B)^{-1}B\right\| \frac{\varepsilon}{\sqrt{1-\varepsilon^2}} + O\left(\varepsilon^2\right).$$

Therefore, it follows from above and the Taylor expansion on $\sqrt{1-\varepsilon^2}$ that (15) holds. ∎

REMARK. Inequality (14) indicates that in the global sense the refined shift-and-invert Arnoldi method converges, though it may converge extremely slowly because of the factor $1/m$. However, it is shown in [12] that generally this factor cannot be removed without additional assumption. If $\tilde{\theta}_i$ is simple and not too ill-conditioned, then (15) shows that the refined method converges with the linear rate in ε. Note that $\varepsilon \to 0$ is a necessary condition for convergence of all projection type methods [2,10]. So it is a natural hypothesis when considering convergence of a projection method. Therefore, the refined method corrects the possible nonconvergence of the shift-and-invert Arnoldi method. For more details on the convergence of general refined projection methods and of refined Ritz vectors, we refer to [11,12,17,19].

5. PRACTICAL IMPLEMENTATIONS

Ruhe has provided a shifted and inverted Arnoldi program for MATLAB 5.0 (see `sptarn.m` in the PDE toolbox in MATLAB). It computes all the eigenvalues and the associated eigenvectors in a rectangle in the complex plane with opposite corners given by the two complex numbers lb and ub. When no more eigenvalues are found in the region $[lb, ub]$, the program stops.

The code used in our experiments for Algorithm 1 is a little different from Ruhe's. We make some modifications to `sptarn.m`. First, we use the subspace spanned by the orthogonalized basis of the converged Ritz vectors instead of the Schur vectors to approximate a desired invariant subspace of the matrix pair (A, B). The orthogonalized basis can be obtained by small-sized QR decompositions. For the refined shift-and-invert Arnoldi algorithm, accordingly, we use the subspace spanned by the orthogonalized basis of the converged refined Ritz vectors to approximate the desired invariant subspace. Second, at each restart of our programs, we select a Ritz vector or a refined Ritz vector associated with the first Ritz value in the region $[lb, ub]$ that has not yet converged. Then the new initial vector is constructed by orthogonalizing the Ritz vector or the refined Ritz vector to all those converged approximate eigenvectors found. Since we cannot know how many eigenvalues there are in the given rectangle in practical computation in advance, our programs stop whenever the number of approximate eigenpairs found is bigger than or equal to a given number k. This avoids the programs running endlessly as Ruhe's code may do. As a consequence, the eigenvalues computed lie in the region $[lb, ub]$ if the number of eigenvalues in $[lb, ub]$ is bigger than k; otherwise, some of the eigenvalues computed are outside this region if the number of eigenvalues in the region is smaller than k.

In our programs, the matrix by vector products $(A - \sigma B)^{-1}x$ is computed by two steps. First, we use the MATLAB `lu` command to obtain the sparse LU factors of the matrix $A - \sigma B$; then $(A - \sigma B)^{-1}x = U\backslash L\backslash x$, where the backslash is the MATLAB left matrix divide command.

Finally, we offer a few words about how to test convergence. In experiments, based on (8) and (12), we claim that Algorithm 1 has converged when

$$h_{m+1,m}\,|e_m^* \tilde{y}_i| \le \text{tol}, \tag{16}$$

and that Algorithm 2 has converged when

$$\sigma_{\min}\left(\tilde{H}_m - \tilde{\theta}_i \tilde{I}_m\right) \le \text{tol}, \tag{17}$$

where tol is a user prescribed tolerance. In such a way, we do not need to form the Ritz vector $\tilde{\varphi}_i$ and the refined Ritz vector $\tilde{u}_i$ before they converge.

6. NUMERICAL EXPERIMENTS

We have tested the shift-and-invert Arnoldi algorithm and the refined shift-and-invert Arnoldi algorithm using MATLAB 5.0 on an INTEL PENTIUM 450 MHz with the machine precision eps $\approx 2.22 \times 10^{-16}$. In the experiments, we used the function **sparse** in MATLAB 5.0 to save the matrix

in question, so that only the nonzero entries of the matrix enter the computation of matrix by vector products.

EXAMPLE 1. Consider the Tolosa matrix pair (A, B) from aerodynamics related to the stability analysis of a model of a plane in flight [1]. Here A is a sparse and highly nonnormal matrix with the order $N = 2000$ and B is an identity matrix with the same order. Since the eigenproblem of (A, B) is very ill-conditioned, it can be very difficult to compute a few eigenpairs of it.

We were interested in the eigenvalues close to the origin. Set a region $[lb, ub]$ with $lb = -15 - i$ and $ub = -1 + 15i$. We selected different shifts σ and computed 23 eigenpairs of (A, B) in this region. Algorithms 1 and 2 were stopped as soon as stopping criteria (16) and (17) are satisfied for $(\tilde{\lambda}_i, \tilde{\varphi}_i)$ and $(\tilde{\lambda}_i, \tilde{u}_i)$, $i = 1, 2, \ldots, k$, respectively, where tol $= 10^{-8}$. They used the same initial vector v_1 generated randomly in a uniform distribution. Table 1 shows the results, where "Iter." denotes the number of restarts, "CPU" the CPU timings in seconds, and "n.c." failure to compute all the desired eigenvalues.

Table 1. Results of Example 1.

		SIA		RSIA	
m	σ	Iter.	CPU	Iter.	CPU
30	−12.05	7	70.2	5	53.7
35	−12.05	3	31.7	3	32.0
40	−12.05	2	29.3	2	29.9
45	−12.05	3	55.6	2	39.1
50	−12.05	2	46.3	2	47.5
30	−11.5	500	n.c.	27	287.5
35	−11.5	11	138.5	7	78.0
40	−11.5	6	81.7	5	75.4
45	−11.5	4	65.7	3	50.0
50	−11.5	3	63.3	3	57.9
35	−11	500	n.c.	18	236
40	−11	8	118	6	87.6
45	−11	5	91.2	4	71.5
50	−11	3	58.1	3	59.1
35	−10.5	500	n.c.	41	576
40	−10.5	500	n.c.	9	169
45	−10.5	6	109	5	92.0
50	−10.5	4	82.7	3	59.1
35	−10	500	n.c.	85	1225
40	−10	500	n.c.	20	326
45	−10	11	229	8	152
50	−10	4	82.7	4	109

It is seen from Table 1 that Algorithm 2 was much more efficient than Algorithm 1 in many cases in terms of CPU timings and the number of restarts. Only for quite large m and well-selected shifts σ, e.g., $m = 45, 50$ and $\sigma = -12.05$, Algorithm 1 was comparable to Algorithm 2. When $\sigma = -11, -10.5, -10$ and $m = 35, 40$, Algorithm 1 failed to find all the desired eigenvalues, while Algorithm 2 worked successfully.

EXAMPLE 2. Consider the constant coefficient convention diffusion differential equation

$$-\Delta u(x, y) + p_1 u_x(x, y) + p_2 u_y(x, y) - p_3 u(x, y) = \lambda u(x, y) \tag{18}$$

on a square region $[0,1] \times [0,1]$ with the boundary condition $u(x,y) = 0$, where p_1, p_2, and p_3 are positive constants. Discretization by five point difference on uniform $n \times n$ grid points using the rowwise natural ordering gives a block tridiagonal matrix of the form

$$A = \begin{pmatrix} T & (\beta+1)I & & & \\ (-\beta+1)I & T & (\beta+1)I & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & (\beta+1)I \\ & & & (-\beta+1)I & T \end{pmatrix} \tag{19}$$

with

$$T = \begin{pmatrix} 4-\tau & \gamma-1 & & & \\ -\gamma-1 & 4-\tau & \gamma-1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \gamma-1 \\ & & & -\gamma-1 & 4-\tau \end{pmatrix}, \tag{20}$$

where $\beta = (1/2)p_1 h$, $\gamma = (1/2)p_2 h$, $\tau = p_3 h^2$, and $h = 1/(n+1)$. The order of A is $N = n^2$.

By taking $p_1 = 1$, $p_2 = p_3 = 0$, and $n = 30$, we can obtain a 900×900 matrix $A(30)$. Let B be the identity matrix with order 900. Algorithms 1 and 2 were run on the matrix pair $(A(30), B)$. Set a region $5 < \mathrm{Re}(\lambda) < 7$. We wanted to compute 20 eigenvalues close to the shift $\sigma = 6$. In the experiments, all the v_1s were the same, and the stopping requirement and the notation used were as before. Table 2 lists the results.

Table 2. Results of Example 2.

	SIA		RSIA	
m	Iter.	CPU	Iter.	CPU
30	500	n.c.	41	116
35	500	n.c.	21	84.6
40	149	653	14	67.1
45	29	152	9	50.9
50	5	32.6	4	27.5

We can see from Table 2 that Algorithm 2 made great improvements over Algorithm 1. Only for quite large m, e.g., $m = 50$, Algorithm 1 was comparable to Algorithm 2. When $m = 30, 35$, Algorithm 1 did not compute all the desired eigenvalues, while Algorithm 2 performed efficiently.

EXAMPLE 3. Dielectric channel waveguide problems arise in many integrated circuit applications. Discretization of the governing Helmholtz equation for the magnetic field H

$$\nabla^2 H_x + k^2 n^2(x,y) H_x = \beta^2 H_x, \tag{21}$$

$$\nabla^2 H_y + k^2 n^2(x,y) H_y = \beta^2 H_y \tag{22}$$

by finite difference leads to an unsymmetric matrix eigenvalue problem of the form

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix} = \beta^2 \begin{pmatrix} B_{11} & \\ & B_{22} \end{pmatrix} \begin{pmatrix} H_x \\ H_y \end{pmatrix}, \tag{23}$$

where C_{11} and C_{22} are five- or tri-diagonal matrices, C_{12} and C_{21} are (tri-)diagonal matrices, and B_{11} and B_{22} are nonsingular diagonal matrices.

Table 3. Results of Example 3.

	SIA		RSIA	
m	Iter.	CPU	Iter.	CPU
30	500	n.c.	488	510
40	500	n.c.	197	386
50	353	1118	67	202
60	152	640	50	215
70	181	1017	38	218
80	124	918	26	192
90	59	532	22	199

Table 4. Results of Example 4.

		SIA		RSIA	
m	σ	Iter.	CPU	Iter.	CPU
30	−3.5	500	n.c.	15	13.0
35	−3.5	112	128	9	10.0
40	−3.5	500	n.c.	5	7.3
45	−3.5	6	12.1	3	5.5
50	−3.5	5	11.9	3	6.4
30	−3	500	n.c.	12	10.4
35	−3	500	n.c.	7	7.9
40	−3	500	n.c.	4	5.8
45	−3	7	11.6	4	6.9
50	−3	3	7.3	2	4.6
30	−2.9	500	n.c.	9	8.0
35	−2.9	500	n.c.	7	7.9
40	−2.9	500	n.c.	6	8.3
45	−2.9	6	11.6	2	4.0
50	−2.9	2	4.1	2	4.6
30	−2.5	500	n.c.	10	8.5
35	−2.5	496	480	4	4.7
40	−2.5	7	9.2	3	5.3
45	−2.5	2	3.6	2	3.9
50	−2.5	1	2.4	1	2.9

We tested the problem with $N = 2048$ and computed 20 eigenvalues close to the shift $\sigma = 0.98$. We take the region $-10 < \mathrm{Re}(\lambda) < 10$. Here, all the v_1s were the same, and the stopping requirement and the notation used were as Example 1. Table 3 shows the results.

It is seen from Table 3 that Algorithm 2 had a considerable improvement over Algorithm 1, as shown by Iter. and CPU. Besides, we found that Algorithm 1 with $m = 70$ used more restarts than that with $m = 60$. This is not surprising since from the theoretical analysis [10,13], a larger m does not necessarily give better Ritz vectors than a smaller m does, so that a new initial v_1 in the next restart may not contain more information on the required eigenvectors and thus slowed down the convergence.

EXAMPLE 4. This example is a generalized matrix eigenvalue problem arising in the modal analysis of dissipative magnetohydrodynamics (MHD) [1]. The MHD system combines Maxwell's and fluid flow equations. The physical objective of these MHD systems is to derive nuclear energy from the fusion of light nuclei. The plasmas generated exhibit both the characteristics of an ordinary fluid and special features caused by the magnetic field. The resulting MHD equations

are solved by applying the Galerkin method in conjunction with finite elements, which leads to the generalized eigenvalue problems. The corresponding eigenproblem comprises complicated eigenvalue patterns having different orders of magnitude corresponding to the very different time scales of the behavior involved in the system. We took the matrix pair (A, B) with order $N = 416$ from [1], and computed the 15 eigenvalues of $A\varphi = \lambda B\varphi$ around the different shifts $\sigma = -3.5, -3, -2.9, -2.5$ in the region $[lb, ub]$ with $lb = -5 - 50i$ and $ub = 5 + 50i$. Table 4 reports the results computed. In stopping criteria (16) and (17), we took tol $= 10^{-6}$.

It is observed that Algorithm 2 was much more efficient than Algorithm 1. For nearly half of the cases tested, Algorithm 1 failed to computed all the required eigenvalues, but Algorithm 2 worked very well for all the cases.

In summary, our refined Algorithm 2 can outperform Algorithm 1 very much. By making additional modifications, it should be extended to the rational Krylov algorithms presented by Ruhe [6–9]. We would expect that the resulting refined algorithms are more efficient.

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