Weighted Harmonic Arnoldi Method for Large Interior Eigenproblems

Zhengsheng Wang, Jing Qi, Chuntao Liu, Yuanjun Li

Abstract—The harmonic Arnoldi method can be used to find interior eigenpairs of large matrices. However, it has been shown that this method may converge erratically and even may fail to do so. In this paper, we present a new method for computing interior eigenpairs of large nonsymmetric matrices, which is called weighted harmonic Arnoldi method. The implementation of the method has been tested by numerical examples, the results show that the method converges fast and works with high accuracy.

Keywords—Harmonic Arnoldi method, Weighted Harmonic Arnoldi method, Eigenpair, Interior eigenproblem, Nonsymmetric matrix.

I. Introduction

CONSIDER the large interior eigenvalue problem

$$Ax_i = \lambda_i x_i \qquad (1)$$

where A is an $n \times n$ real matrix, and (λ_i, x_i) is referred to as an eigenpair of A with $\|x_i\| = 1, i = 1, 2, \cdots, n$. Here the norm used is the Euclidean norm. We are mainly interested in computing some interior eigenpairs of A.

Recently, interior eigenvalue problems have been receiving a lot of attention. Eigenvalues in the middle of the spectrum are required for studying tidal motion, and for both adaptive polynomial preconditioning and Richardsons iteration for indefinite systems of linear equations. Other implementations include power system simulations and stability analysis in computational fluid dynamics [1], [4], and so on. In this paper we assume that factorization is impractical for the size and structure of the matrix. This makes the problem difficult.

For the given target point τ, interior eigenvalue problems mean that we want to compute some eigenvalues near τ. Note that

$$(A - \tau I)^{-1} x_i = \frac{1}{\lambda_i - \tau} x_i \qquad (2)$$

Zhengsheng Wang: Department of Mathematics, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China. e-mail: wangzhengsheng@nuaa.edu.cn

Jing Qi: Department of Mathematics, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China. e-mail: qijingmath@163.com

Chuntao Liu: Department of Mathematics, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China. e-mail: liuchuntao9@126.com

Yuanjun Li: Department of Mathematics, Nanjing University of Aeronautics and Astronautics, Nanjing 210016, P. R. China. e-mail: lyj861125@163.com

So the eigenvalues near τ are transformed into exterior ones. Here the eigenvalues $\lambda_1, \cdots, \lambda_n$ of A are ordered by increasing real parts or magnitude from τ.

When $(A - \tau I)^{-1} v$ can be computed, the shift-invert Arnoldi method[12] is one of the most effective methods for solving interior eigenvalue problems (2). Further, when A is too large to factor, one can use the inexact shift-invert Arnoldi algorithm, that is, matrix-vector products $(A - \tau I)^{-1} v$ can be computed by solving the system $(A - \tau I)u = v$ approximately using an iterative method such as GMRES. However, as assumed, factoring $A - \tau I$ is impractical. So we abandon this idea here.

The harmonic Arnoldi method[1], [2], [3], [4] is one kind of projection method for solving the interior eigenvalue problem. A remarkable merit of the harmonic Arnoldi method is that it is suitable for computing interior eigenvalues and associated eigenvectors of A since it transforms interior eigenvalues into exterior ones without factoring $A - \tau I$.

Like the standard projection methods, to improve efficiency and limit memory requirements, the harmonic Arnoldi methods are restarted after m iterations, and the method of restart is crucial for the success and efficiency of a restarted algorithm. The implicit restart approach has appeared to be a very useful technique. A key for the success of the implicit restart technique is reasonable selection of shifts. The implicitly restarted harmonic Arnoldi algorithm by Morgan[3] most often used those unwanted harmonic Ritz values as shifts.

The weighted Arnoldi method is a quite effective scheme for large eigenvalue problems[5]. In this paper, we apply the weighted techniques to the harmonic Arnoldi method for the large interior eigenvalue problems, so called a weighted harmonic Arnoldi method.

The outline of this paper is as follows. In Section 2, we review the harmonic Arnoldi method. In Section 3, a weighted harmonic Arnoldi method is proposed. In Section 4, some numerical experiments and comparisons are given which show that this new method is powerful and cost effective scheme for computing large matrix interior eigenvalue problems. Finally, we make some concluding remarks.

Throughout the paper, denote by $K_m(A, v)$ the Krylov subspace spanned by $v, Av, A^2 v, \cdots, A^{m-1} v$, A^T denote the transpose matrix of A and A^H denote the conjugate transpose matrix of A.

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II. THE HARMONIC ARNOLDI METHOD

Assume $dim(K_m(A, v_1)) = m$. The Arnoldi process builds up an orthonormal basis $\{v_i\}_{i=1}^m$ of $K_m(A, v_1)$, and it can be written in the matrix form

$$AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^* = V_{m+1} \widetilde{H}_m \quad (3)$$

where e_m^* is the mth coordinate vector of dimension m, $V_m = [V_m, v_{m+1}] = [v_1, v_2, \cdots, v_{m+1}]$ is an $n \times (n+1)$ matrix whose columns form an orthonormal basis of the $(m+1)$-dimensional Krylov subspace $K_{m+1}(A, v_1)$, and $\widetilde{H}_m$ is the $(m+1) \times m$ upper Hessenberg matrix which is the same as H_m except for an additional row whose only nonzero entry is $h_{m+1,m}$ in position $(m+1, m)$.

For the given target point τ in (2), the harmonic Arnoldi method seeks the pairs $(\widetilde{\lambda}_i, \widetilde{x}_i)$ satisfying the harmonic projection[3]

$$\begin{cases} \widetilde{x}_i \in K_m(A, v_1) \\ (A - \tau I)\widetilde{x}_i - (\widetilde{\lambda}_i - \tau)\widetilde{x}_i \perp (A - \tau I)K_m(A, v_1) \end{cases} \quad (4)$$

and uses them to approximate some eigenvalues of A near τ and the associated eigenvectors. $(\widetilde{\lambda}_i, \widetilde{x}_i)$ are called harmonic Ritz values and harmonic Ritz vectors of A with respect to $K_m(A, v_1)$, respectively. It is seen from (3) that the above procedure is equivalent to solving the generalized eigenproblem

$$\begin{cases} \widetilde{x}_i = V_m g_i \\ (H_m - \tau I_m)^H g_i = \frac{1}{\widetilde{\lambda}_i - \tau}(\widetilde{H}_m - \tau \widetilde{I}_m)^H (\widetilde{H}_m - \tau \widetilde{I}_m) g_i \end{cases} \quad (5)$$

where $\widetilde{I}$ is the $(m+1) \times m$ identity matrix with the last row being zero.

The algorithm can be presented as follows.

Algorithm 2.1 The harmonic Arnoldi Method

1) Start: Given the dimension of a Krylov subspace m, the target point τ, the number k $(k < m)$ of desired eigenpairs, and a prescribed tolerance tol. Choose an initial vector v_1 with unit length;
2) Iteration: Construct the upper Hessenberg matrices H_m and $\widetilde{H}_m$ as well as V_m by the Arnoldi process;
3) Computation of approximate eigenpairs $(\widetilde{\lambda}_i, \widetilde{x}_i), (i = 1, 2, \cdots, m)$ by:
   if $H_m - \tau I$ is singular, solving

$$[(H_m - \tau I) + (H_m - \tau I)^{-H} e_m h_{m+1,m}^H h_{m+1,m} e_m^H] g_i$$
$$= (\widetilde{\lambda}_i - \tau) g_i$$

   otherwise, solving

$$[(H_m - \tau I)^H (H_m - \tau I) e_m h_{m+1,m}^H h_{m+1,m} e_m^H] g_i$$
$$= (\widetilde{\lambda}_i - \tau)(H_m - \tau I)^H g_i$$

Then select the k pairs $(\widetilde{\lambda}_i, \widetilde{x}_i)$ as approximations to the wanted eigenpairs (λ_i, x_i) where $\widetilde{x}_i = V_m g_i, i = 1, 2, \cdots, k$;
4) Test for convergence: Compute the residual norms of $(\widetilde{\lambda}_i, \widetilde{x}_i)$ directly, $i = 1, 2, \cdots, k$. If thet are all below the tol, then stop, else continue;
5) Restart: Using the harmonic Ritz vector $\widetilde{x}_i, i = 1, 2, \cdots, k$ to form a new initial vector v_1, and go to step 2.

III. THE WEIGHTED HARMONIC ARNOLDI METHOD

We define the D-scalar product as

$$(u, v)_D = v^T D u \quad (6)$$

$$(u, v)_D = v^T D u = \sum_{i=1}^n d_i u_i v_i \quad (7)$$

where $D = diag[d_1, d_2, \cdots, d_n], d_i > 0$, u and v are two vector. Also, denote $d = [d_1, d_2, \cdots, d_n]^T$.

The norm associated with this inner product is the D-norm $\| \cdot \|_D$ and defined by $\| \cdot \|_D = \sqrt{(u, u)_n} = \sqrt{u^T D u} = \sqrt{\sum_{i=1}^n d_i u_i^2}$. We choose the vector d such that $\|d\|_2 = \sqrt{n}$. This choice enables us to recover the Euclidean norm if all the elements of d are equal.

The following algorithm describes the weighted Arnoldi process which uses the D-inner product $(\cdot, \cdot)_D$ to construct a D-orthonormal basis of $K_m(A, v)$ starting with the vector $\widetilde{v}_1 = \frac{v}{\|v\|_D}$. The aim of defining the new inner product is moving components of residual vector to zero as fast as possible cases.

Algorithm 3.1 The weighted Arnoldi process

1) Start: Choose an initial vector $\widetilde{v}_1$ such that $\widetilde{v}_1 = \frac{v}{\|v\|_D}$;
2) Iteration: For $j = 1, 2, \cdots, m$, do

$$w = A\widetilde{v}_j$$

for $i = 1, 2, \cdots, j$, do

$$w = w - \widetilde{h}_{ij}\widetilde{v}_i$$

$$\widetilde{h}_{j+1,j} = \|w\|_D; \widetilde{v}_{j+1} = \frac{w}{\widetilde{h}_{j+1,j}}$$

Vectors $\widetilde{v}_1, \widetilde{v}_2, \cdots, \widetilde{v}_m$ generated by Algorithm 2 form a D-orthonormal base, in other words, if $\widetilde{V}_m = [\widetilde{v}_1, \widetilde{v}_2, \cdots, \widetilde{v}_m]$, then $\widetilde{V}_m D \widetilde{V}_m^T = I_m$.

Theorem 3.1 *If $\widetilde{H}_m \in R^{n \times n}$ is the upper Hessenberg matrix constructed by weighted Arnoldi process, then*
$(1) A\widetilde{V}_m = \widetilde{V}_m \widetilde{H}_m + \widetilde{h}_{m+1,m} \widetilde{v}_{m+1} e_m^T,$
$(2) \widetilde{V}_m^T D A \widetilde{V}_m \approx \widetilde{H}_m$
Najafi has given the proof in [5].

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Then, we give a weighted harmonic Arnoldi method for large interior eigenproblems presented as follows.

Algorithm 3.2 The weighted harmonic Arnoldi Method

1) Start: Given the dimension of a Krylov subspace m, the target point τ, the number k $(k < m)$ of desired eigenpairs, and a prescribed tolerance tol. Choose an initial vector v_1 with unit length and vector d with $\|d\|_2 = \sqrt{n}$;

2) Iteration: Construct the upper Hessenberg matrices $\widetilde{H}_m$ as well as $\widetilde{V}_{m+1} = [\widetilde{v}_1, \widetilde{v}_2, \cdots, \widetilde{v}_{m+1}]$ by the weighted Arnoldi process with the initial vector $\widetilde{v}_1 = \frac{v_1}{\|v_1\|_D}$;

3) Computation of approximate eigenpairs $(\widetilde{\lambda}_i, \widetilde{x}_i), (i = 1, 2, \cdots, m)$ by:
   if $\widetilde{H}_m - \tau I$ is singular, solving

$$[(\widetilde{H}_m - \tau I) + (\widetilde{H}_m - \tau I)^{-H} e_m \widetilde{h}_{m+1,m}^H \widetilde{h}_{m+1,m} e_m^H] g_i$$
$$= (\widetilde{\lambda}_i - \tau) g_i$$

otherwise, solving

$$[(\widetilde{H}_m - \tau I)^H (\widetilde{H}_m - \tau I) e_m \widetilde{h}_{m+1,m}^H \widetilde{h}_{m+1,m} e_m^H] g_i$$
$$= (\widetilde{\lambda}_i - \tau)(\widetilde{H}_m - \tau I)^H g_i$$

Then select the k pairs $(\widetilde{\lambda}_i, \widetilde{x}_i)$ as approximations to the wanted eigenpairs (λ_i, x_i) where $\widetilde{x}_i = \widetilde{V}_m g_i, i = 1, 2, \cdots, k$;

4) Test for convergence: Compute the residual vector r_i of $(\widetilde{\lambda}_i, \widetilde{x}_i)$ directly, $i = 1, 2, \cdots, k$, if the residual norms are all below the tol, then stop; else, denote r_0 is the minimal residual vector such that $\|r_0\|_2 = min_{1 \leq i \leq m} \|r_i\|_2$; compute $d_i = \sqrt{n} \frac{|(r_0)_i|}{\|r_0\|_2}$, $d = [d_1, d_2, \cdots, d_n]$, continue.

5) Restart: Using the harmonic Ritz vector $\widetilde{x}_i, i = 1, 2, \cdots, k$ to form a new initial vector $\widetilde{v}_1$, and go to step 2.

IV. NUMERICAL EXPERIMENTS

In this section we report some numerical experiments on four problems. We have tested all the algorithms using MAT-LAB 6.5 on a Intel Centrino 2 GHz with main memory 1024M and machine precision $\varepsilon = 2.22 \times 10^{-16}$. To make a fair and reasonable comparison, for each example, the same vector was generated randomly in a uniform distribution, orthogonalized and utilized as the initial guess. The algorithms stopped as soon as

$$max_{1 \leq i \leq k} \|(A - \widetilde{\lambda}_i I) \widetilde{x}_i\|_2 \leq tol$$

In all the tables below, we denote by m the steps of the Arnoldi process, by $iter$ the number of restarting, by err the residual norm error, and by CPU the CPU timings in seconds.

Example 4.1 This problem is from [10], and the data file is DW2048 in MATLAB. We are interested in finding the three leftmost eigenpairs, i.e., the eigenvalues with three smallest real parts.

We ran Algorithm 1 and Algorithm 3 on this problem. The algorithms stopped as soon as the residual norm dropped below $tol = 1e - 6$. The three approximate eigenvalues calculated were $\widetilde{\lambda}_1 \approx -0.62551291$, $\widetilde{\lambda}_2 \approx -0.61442057$, $\widetilde{\lambda}_3 \approx -0.59673082$. Table 1 reports the results obtained.

TABLE I: COMPARISON OF THE TWO METHODS
WITH MATRIX DW2048

$DW2048$	$Algorithm1$			$Algorithm3$		
m	$iter$	CPU	err	$iter$	CPU	err
20	429	26.5	1.0566e-6	78	5.9	2.3427e-7
30	35	3.7	1.2712e-7	12	1.6	1.5396e-8
40	20	4.1	2.2248e-7	4	3.1	5.1877e-10

For this example, it was shown that Algorithm 3 (weighted harmonic Arnoldi method) worked much better than Algorithm 1 (harmonic Arnoldi method), especially when m was relatively small. When the dimension of the Krylov subspace is bigger and bigger, the iterations of the two algorithms become less and less. However, the error of the weighted Arnoldi method is better.

Example 4.2 This example is taken from the Harwell-Boeing Sparse Matrix Collection. We tested three matrices BP1000, BP1400 and BP1600. They are of order 822. We are interested in finding the three leftmost eigenpairs of each matrix, i.e., the eigenvalues with three smallest real parts.

We ran Algorithm 1 and Algorithm 3 on this problem. The algorithms stopped as soon as the residual norm dropped below $tol = 1e - 6$. Table 2, Table 3 and Table 4 report the results obtained.

TABLE II: COMPARISON OF THE TWO METHODS
WITH MATRIX BP1000

$BP1000$	$Algorithm1$			$Algorithm3$		
m	$iter$	CPU	err	$iter$	CPU	err
20	106	5.5	1.7180e-7	72	3.6	3.7135e-10
30	7	0.7	4.8156e-7	6	0.4	7.7592e-9
40	5	0.3	5.7260e-8	3	0.2	1.4285e-12

TABLE III: COMPARISON OF THE TWO METHODS
WITH MATRIX BP1400

$BP1400$	$Algorithm1$			$Algorithm3$		
m	$iter$	CPU	err	$iter$	CPU	err
30	219	9.5	3.6077e-7	32	3.2	5.4518e-8
40	8	1.7	1.2865e-7	3	1.2	1.2148e-9
50	5	1.3	2.4686e-8	2	1.1	5.8912e-12

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TABLE IV: COMPARISON OF THE TWO METHODS
WITH MATRIX BP1600

$BP1600$	$Algorithm1$			$Algorithm3$		
m	$iter$	CPU	err	$iter$	CPU	err
30	211	9.7	7.3054e-7	69	4.6	1.9535e-8
40	8	1.6	1.0287e-8	5	1.2	4.3004e-11
50	3	1.1	1.3194e-8	2	1.1	1.9592e-13

For this example, it also was shown that Algorithm 3 (weighted harmonic Arnoldi method) worked much better than Algorithm 1 (harmonic Arnoldi method), especially when m was relatively small. When the dimension of the Krylov subspace is bigger and bigger, the iterations of the two algorithms become less and less. However, the error of the weighted Arnoldi method is better.

V. CONCLUSION AND REMARKS

In this paper, we proposed a weighted harmonic Arnoldi method for large interior eigenproblems. Numerical examples indicate that the new method often performs much better than the original harmonic Arnoldi method. Furthermore, we would like to point out that the strategy presented in this paper may also be combined with other Krylov subspace methods, such as Jacobi-Davidson and block methods. We expect the resulting algorithms were more powerful. Those need further research.

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