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

\[ Ax_i = \lambda_i x_i \]  

(1)

where \( A \) is an \( n \times n \) real matrix, and \((\lambda_i, x_i)\) is referred to as an eigenpair of \( A \) with \( \|x_i\| = 1, i = 1, 2, \ldots, n \). 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 Richardsions 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 limit memory requirements, the harmonic 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.

So the eigenvalues near \( \tau \) are transformed into exterior ones. Here the eigenvalues \( \lambda_1, \ldots, \lambda_n \) of \( A \) are ordered by increasing real parts or magnitude from \( \tau \).

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.

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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 \( v, A v, A^2 v, \ldots, A^{m-1} v \), \( A^T \) denote the transpose matrix of \( A \) and \( A^H \) denote the conjugate transpose matrix of \( A \).
II. THE HARMONIC ARNOLDI METHOD

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

\[
AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^* = V_{m+1} \tilde{H}_m \tag{3}
\]

where \( e_m^* \) is the \( m \)-th coordinate vector of dimension \( m \), \( V_m = [v_1, v_2, \cdots, v_{m+1}] \) is an \( n \times (m+1) \) matrix whose columns form an orthonormal basis of the \((m+1)\)-dimensional Krylov subspace \( K_{m+1}(A, v_1) \), and \( H_m \) 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 \( \tau \) in (2), the harmonic Arnoldi method seeks the pairs \((\tilde{\lambda}_i, \tilde{x}_i)\) satisfying the harmonic projection[3]

\[
\begin{align*}
\tilde{x}_i & \in K_m(A, v_1) \\
(A - \tau I) \tilde{x}_i - (\tilde{\lambda}_i - \tau) \tilde{x}_i & \perp (A - \tau I) K_m(A, v_1)
\end{align*}
\tag{4}
\]

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

\[
\begin{align*}
\tilde{x}_i & = V_m g_i \\
(H_m - \tau I_m)^H g_i & = \frac{1}{\tilde{\lambda}_i - \tau} (\tilde{H}_m - \tau \tilde{I}_m)^H (\tilde{H}_m - \tau \tilde{I}_m) g_i
\end{align*}
\tag{5}
\]

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

Then select the \( k \) pairs \((\tilde{\lambda}_i, \tilde{x}_i)\) as approximations to the wanted eigenpairs \((\lambda_i, x_i)\) where \( \tilde{x}_i = V_m g_i, i = 1, 2, \cdots, k; \)

4) Test for convergence: Compute the residual norms of \((\tilde{\lambda}_i, \tilde{x}_i)\) directly, \( i = 1, 2, \cdots, k \). If they are all below the tol, then stop, else continue;

5) Restart: Using the harmonic Ritz vector \( \tilde{x}_i, i = 1, 2, \cdots, k \) 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

\[
(u, v)_D = v^T D u
\tag{6}
\]

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

where \( D = \text{diag}(d_1, d_2, \cdots, d_n) \), \( d_i > 0 \), \( u \) 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 \( \| \cdot \|_D = \sqrt{(u, u)_D} = \sqrt{u^T D u} = \sqrt{\sum_{i=1}^n d_i u_i^2} \). 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 \( \tilde{v}_1 = \frac{v}{\|v\|_D} \).

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: Given the dimension of a Krylov subspace \( m \), the target point \( \tau \), 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 \( \tilde{H}_m \) as well as \( V_m \) by the Arnoldi process;

3) Computation of approximate eigenpairs \((\tilde{\lambda}_i, \tilde{x}_i), (i = 1, 2, \cdots, m)\) by :

if \( H_m - \tau I \) is singular, solving

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

otherwise, solving

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

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

Theorem 3.1 If \( \tilde{H}_m \in \mathbb{R}^{n \times n} \) is the upper Hessenberg matrix constructed by weighted Arnoldi process, then

\[
1) \tilde{A} \tilde{V}_m = \tilde{V}_m \tilde{H}_m + \tilde{h}_{m+1,m} \tilde{v}_{m+1} e_m^T
\]

\[
2) \tilde{V}_m^T D \tilde{A} \tilde{V}_m \approx \tilde{H}_m
\]

Najafi has given the proof in [5].
Then, we give a weighted harmonic Arnoldi method for large interior eigenproblems as presented as follows.

Algorithm 3.2 The weighted harmonic Arnoldi Method

1) Start: Given the dimension of a Krylov subspace \( m \),
the target point \( \tau \), 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
\[ \|d\|_2 = \sqrt{m}; \]
2) Iteration: Construct the upper Hessenberg matrices \( \tilde{H}_m \)
as well as \( \tilde{V}_{m+1} = [\tilde{v}_1, \tilde{v}_2, \ldots, \tilde{v}_{m+1}] \) by the weighted
Arnoldi process with the initial vector \( \tilde{v}_1 \Rightarrow \frac{v_1}{\|v_1\|_D} \);
3) Computation of approximate eigenpairs \((\tilde{\lambda}_i, \tilde{x}_i)\), \(i = 1, 2, \ldots, m\) by;
   - if \( \tilde{H}_m - \tau I \) is singular, solving
   \[
   (\tilde{H}_m - \tau I) + (\tilde{H}_m - \tau I)^H \tilde{e}_m \tilde{H}_m + \tilde{e}_m^2 \tilde{H}_m^2 g_i
   = (\tilde{\lambda}_i - \tau)g_i
   \]
   otherwise, solving
   \[
   (\tilde{H}_m - \tau I)H \tilde{e}_m = \tilde{H}_m + \tilde{H}_m^2 \tilde{H}_m^2 g_i
   = (\tilde{\lambda}_i - \tau)(\tilde{H}_m - \tau I)^H g_i
   \]
Then select the \( k \) pairs \((\tilde{\lambda}_i, \tilde{x}_i)\) as approximations to
the wanted eigenpairs \((\lambda_i, x_i)\) where \( \tilde{x}_i = \tilde{V}_mg_i, i = 1, 2, \ldots, k \);
4) Test for convergence: Compute the residual vector \( r_i \) of
\((\tilde{\lambda}_i, \tilde{x}_i)\) directly, \(i = 1, 2, \ldots, k\), if the residual norms are
all below \( tol \), then stop; else, denote \( r_0 \) is the min-
imal residual vector such that \( \|r_0\|_2 = \min_{1 \leq i \leq k} \|r_i\|_2 \); compute
\( d_i = \sqrt{\frac{\|r_0\|_2}{\|r_0\|^2}} \), \( d = [d_1, d_2, \ldots, d_k] \), continue.
5) Restart: Using the harmonic Ritz vector \( \tilde{x}_i, i = 1, 2, \ldots, k \) to form a new initial vector \( \tilde{v}_1 \), 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 the residual norm dropped below \( tol = 1e-6 \). The three approximate eigenvalues
calculated were \( \lambda_1 \approx -0.62551291, \lambda_2 \approx -0.61442057, \lambda_3 \approx -0.59673082 \). Table 1 reports the results obtained.

TABLE I: COMPARISON OF THE TWO METHODS
WITH MATRIX DW2048

<table>
<thead>
<tr>
<th>DW2048</th>
<th>Algorithm1</th>
<th>Algorithm3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>( \text{iter} )</td>
<td>( \text{CPU} )</td>
</tr>
<tr>
<td>20</td>
<td>429</td>
<td>26.5</td>
</tr>
<tr>
<td>30</td>
<td>35</td>
<td>0.7</td>
</tr>
<tr>
<td>40</td>
<td>40</td>
<td>4.1</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>BP1000</th>
<th>Algorithm1</th>
<th>Algorithm3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>( \text{iter} )</td>
<td>( \text{CPU} )</td>
</tr>
<tr>
<td>20</td>
<td>106</td>
<td>5.5</td>
</tr>
<tr>
<td>30</td>
<td>7</td>
<td>0.7</td>
</tr>
<tr>
<td>40</td>
<td>5</td>
<td>0.3</td>
</tr>
</tbody>
</table>

TABLE III: COMPARISON OF THE TWO METHODS
WITH MATRIX BP1400

<table>
<thead>
<tr>
<th>BP1400</th>
<th>Algorithm1</th>
<th>Algorithm3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>( \text{iter} )</td>
<td>( \text{CPU} )</td>
</tr>
<tr>
<td>30</td>
<td>219</td>
<td>9.3</td>
</tr>
<tr>
<td>40</td>
<td>8</td>
<td>1.7</td>
</tr>
<tr>
<td>30</td>
<td>5</td>
<td>1.3</td>
</tr>
</tbody>
</table>
TABLE IV: COMPARISON OF THE TWO METHODS WITH MATRIX BP1600

<table>
<thead>
<tr>
<th>m</th>
<th>BP1600</th>
<th>Algorithm 1</th>
<th>Algorithm 3</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>iter</td>
<td>CPU err</td>
<td>iter</td>
</tr>
<tr>
<td>30</td>
<td>211</td>
<td>9.7 7.3054e-7</td>
<td>69</td>
</tr>
<tr>
<td>40</td>
<td>8</td>
<td>1.6 1.0287e-8</td>
<td>5</td>
</tr>
<tr>
<td>50</td>
<td>3</td>
<td>1.1 1.3194e-8</td>
<td>2</td>
</tr>
</tbody>
</table>

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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