

A New Computational Harmonic Projection Algorithm for Large Unsymmetric Generalized Eigenproblems

H. Saberi Najafi¹, H. Moosaei¹ and M. Moosaei²

¹ Department of Mathematics, Faculty of Sciences
University of Guilan, P.O. Box 41335-1914, Rasht, Iran

² Department of Mathematics, Faculty of Sciences
BuAli Sina University, Hamedan, Iran
hnajafi@guilan.ac.ir, hmoosaei@gmail.com m.moosaei@basu.ac.ir

Abstract

The harmonic projection method can be used to find interior eigenpairs of large matrices. Given a target point or shift σ to which the needed interior eigenvalues are close, the desired interior eigenpairs are the eigenvalues nearest σ and the associated eigenvectors. In this article we use the harmonic projection algorithm for computing the interior eigenpairs of a large unsymmetric generalized eigenvalue problem.

Keywords: Eigenvalue, unsymmetric matrix, harmonic, Arnoldi, shift-and-invert

1 Introduction

The eigenvalue problem is one of the most important subjects in the applied sciences and engineering. One of the most important and practical topics in computational mathematics is computing some of the interior generalized eigenvalues close to target point or shift σ and the associated eigenvectors. Consider the large unsymmetric generalized eigenproblem.

$$CX_i = \theta_i BX_i \quad (1)$$

Where C and B are $N \times N$ large matrices, we are interested in computing some eigenvalues close to a given shift σ and also associated eigenvectors of pair (C,B) . Since the matrices are large the standard numerical methods cannot be used, they are fine for small or medium-size matrices. For computing the

eigenpairs of problem (1) we consider two methods. First method: This is a shift-and-invert Arnoldi method Second method: This is a new computational harmonic projection algorithm

in this paper we comparative first method with second method and the results shown that the first method is better than the second method .

2 Definition

Let A be a $n \times n$ matrix and $v \in R^n$ is a vector, then the subspace generated by vectors $v, Av, \dots, A^{m-1}v$ is called as Krylov subspace and denoted by $k_m(A, v)$, i.e.

$$k_m(A, v) = \text{span}\{v, Av, \dots, A^{m-1}v\}$$

3 Algorithm 1: (Arnoldi MGS process)

Choose a vector v_1 of norm 1

For $j = 1, \dots, m$ do

$w := Av_j$

For $i = 1, \dots, j$ do

$h_{ij} := (w, v_i)$

$w := w - h_{i,j}v_i$

End do

$h_{j+1,j} := \|w\|_2$

$v_{j+1} := \frac{w}{h_{j+1,j}}$

End do.

4 Theorems

Theorem 4.1: The vectors v_1, v_2, \dots, v_m produced by the Arnoldi algorithm form an orthonormal basis of the subspace $k_m = \text{span}\{v_1, Av_1, \dots, A^{m-1}v_1\}$.

Proof in [2].

Theorem 4.2: Denote by V_m a $n \times m$ matrix with column vectors v_1, v_2, \dots, v_m and by H_m a $m \times m$ Hessenberg matrix whose nonzero entries are defined by the algorithm. Then the following relations hold:

$$\begin{aligned} AV_m &= V_m H_m + h_{m+1,m} v_{m+1} e_m^H, \\ V_m^H AV_m &\cong H_m. \end{aligned}$$

Proof in [2].

5 The shift-and-invert Arnoldi method

If the matrix $C - \sigma B$ is invertible for some shift σ , the eigenproblem (1) can be transformed into the standard eigenproblem. $CX_i = \theta_i BX_i$

$$\Rightarrow CX_i - \sigma BX_i = \theta_i BX_i - \sigma BX_i$$

$$\Rightarrow (C - \sigma B)X_i = (\theta_i - \sigma)BX_i$$

$$\Rightarrow \frac{1}{\theta_i - \sigma}X_i = (C - \sigma B)^{-1}BX_i$$

$$\Rightarrow (C - \sigma B)^{-1}BX_i = \frac{1}{\theta_i - \sigma}X_i$$

Now we suppose, $\lambda_i = \frac{1}{\theta_i - \sigma}$ and $A = (C - \sigma B)^{-1}B$ Therefore the problem is:

$$AX_i = \lambda_i X_i \quad (2)$$

It is easy to show that:

the (θ_i, X_i) is eigenpair of problem (1) if and only if (λ_i, X_i) is the eigenpair of problem (2).

Therefore, the shift-and-invert Arnoldi method for 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 $k_m(A, v_1)$ 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 $k_m(A, v_1)$. The approximate solutions for problem (1) can be recovered from these approximate eigenpairs.

By theorem 4.2 the shift-and-invert Arnoldi process can be written in matrix form

$$(C - \sigma B)^{-1}BV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^H$$

or

$$(C - \sigma B)^{-1}BV_m \cong V_{m+1} \tilde{H}_m \quad (3)$$

Where e_m is m^{th} coordinate vector of dimension m , $V_{m+1} = (V_m, v_{m+1}) = (v_1, v_2, \dots, v_{m+1})$ 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 \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 $(\tilde{\lambda}_i, \tilde{y}_i), i = 1, 2, \dots, m$ are the eigenpairs of the matrix H_m ,

$$H\tilde{y}_i = \tilde{\lambda}_i\tilde{y}_i$$

Let $\tilde{\lambda}_i = \frac{1}{\tilde{\theta}_i - \sigma}$ and $\tilde{X}_i = V_m\tilde{y}_i$. (4)

Then the shift-and-invert Arnoldi method uses $(\tilde{\theta}_i, \tilde{X}_i)$ to approximate the eigenpairs (θ_i, X_i) of problem (1). The $\tilde{\theta}_i$ and \tilde{X}_i are called the Ritz values and Ritz vectors of C with respect to $k_m(A, v_1)$, respectively. Define the corresponding residual

$$\tilde{r}_i = (C - \tilde{\theta}_i B)\tilde{X}_i$$

Then we have the following theorem.

Theorem 5.1: The residual \tilde{r}_i corresponding to the approximate eigenpairs $(\tilde{\theta}_i, \tilde{X}_i)$ by the shift-and-invert Arnoldi method satisfy

$$\|\tilde{r}_i\| \leq h_{m+1,m} \left| \tilde{\theta}_i - \sigma \right| \|C - \sigma B\| |e_m^h \tilde{y}_i|$$

proof: From relations (3), (4), we obtain

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

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 l eigenvalues near a target point σ and the associated eigenvectors. We call the resulting algorithm **Algorithm 2**.

6 The new computational harmonic projection algorithm

We have shown in section 4 that the eigenproblem $CX_i = \theta_i BX_i$ can be transformed to the problem $AX_i = \lambda_i X_i$ such that $\theta_i = \frac{1}{\lambda_i} + \sigma$ and $A = (C - \sigma B)^{-1}B$. As we are interested in computing some of the interior eigenvalues close to σ , therefore the large λ_i must be considered.

If τ is large and not to be an eigenvalue of A such that $(A - \tau I)$ is not invertible then we have from $AX_i = \lambda_i X_i$ that

$$(A - \tau I)^{-1}X_i = \frac{1}{\lambda_i - \tau}X_i$$

Therefore, the interior eigenvalues near τ are transformed into exterior ones with largest magnitudes of $(A - \tau I)^{-1}$. For the given τ and a subspace $k_m(A, v)$ the harmonic projection method seeks the pairs $(\tilde{\lambda}_i, \tilde{X}_i)$ satisfying the harmonic projection (for more details see [3, 4]),

$$\begin{cases} \tilde{X}_i \in k_m(A, v_1) & (7a) \\ A\tilde{X}_i - \tilde{\lambda}_i \tilde{X}_i \perp (A - \tau I)k_m(A, v_1) & (7b) \end{cases}$$

and uses them to approximate some eigenvalues of A near τ and the associated eigenvectors.

Theorem 6.1: Let $\tilde{X}_i^{(m)} = V_m g_i^{(m)}$ be the harmonic Ritz vector, $\tilde{\lambda}_i$ be the harmonic Ritz value then:

$$\tilde{r}_i = \left\| (A - \tilde{\lambda}_i^{(m)} I) X_i^{(m)} \right\|$$

Proof: Since we have $AV_m = V_m H_m + h_{m+1,m} v_{m+1} e_m^H$ then

$$AX_i^{(m)} = AV_m g_i^{(m)} = V_m H_m g_i^{(m)} + h_{m+1,m} v_{m+1} e_m^H g_i^{(m)}$$

So

$$\begin{aligned} (A - \tilde{\lambda}_i^{(m)} I) X_i^{(m)} &= AV_m g_i^{(m)} - \tilde{\lambda}_i^{(m)} V_m g_i^{(m)} \\ &= V_m H_m g_i^{(m)} + h_{m+1,m} v_{m+1} e_m^H g_i^{(m)} - \tilde{\lambda}_i^{(m)} V_m g_i^{(m)} \\ &= V_m (H_m - \tilde{\lambda}_i^{(m)} I) g_i^{(m)} + h_{m+1,m} v_{m+1} e_m^H g_i^{(m)} = V_{m+1} \begin{bmatrix} (H_m - \tilde{\lambda}_i^{(m)} I) g_i^{(m)} \\ h_{m+1,m} e_m^H g_i^{(m)} \end{bmatrix}. \end{aligned}$$

Algorithm 3.(The new computational Harmonic projection algorithm)

1. Input, τ , σ , v_1 with $\|v_1\| = 1$, l : the numbers of desired eigenvalues, k : the accuracy, A, B : are $N \times N$ large matrices
2. Set $A = (C - \sigma B)^{-1}B$
3. Run algorithm1. (For computing $V_{m+1} = [v_1, v_2, \dots, v_{m+1}]$ and H_m .)
4. f $H_m - \tau I$ is nonsingular then Solving

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

$$((H_m - \tau I)^H (H_m - \tau I) + e_m h_{m+1,m}^H h_{m+1,m} e_m^H) g_i = (\tilde{\lambda}_i - \tau) (H_m - \tau I)^H g_i$$
 end if;(For computing $(\tilde{\lambda}_i, g_i)$, $i = 1, \dots, m$.)
5. Select $\tilde{\lambda}_i$'s with respect to the smallest value of $(\tilde{\lambda}_i - \tau)$'s is to approximate the desired eigenvalues $i = 1, \dots, l$.
6. Take the harmonic Ritz pairs $(\tilde{\lambda}_i, \tilde{X}_i = V_m g_i)$, $i = 1, \dots, l$ as approximations.
7. Computing $\tilde{r}_i = \|(A - \tilde{\lambda}_i^{(m)} I) \tilde{X}_i^{(m)}\|$ $i = 1, \dots, l$
8. If $\tilde{r}_i = < k$, $i = 1, \dots, l$ then Stop and set $\tilde{\theta}_i = \frac{1}{\tilde{\lambda}_i} + \sigma$ else go to step (9) end;
9. Restarted: use the harmonic Ritz vectors $\tilde{X}_i, i = 1, \dots, l$, for a new initial guess, i.e. v_1 , and go to step 3

7 Numerical experiments

The algorithm has been tested using MATLAB 7.0.1 on a Pentium IV 2.8 GHz with main memory 512 Megabytes. Let C and B are 1001×1001 matrices as

$$C = \begin{bmatrix} -510 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ -1 & -509 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & -1 & -12 & 1 & 0 & 0 & 0 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & -1 & -11 & 1 & 0 & 0 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & 0 & 0 & -1 & 11 & 1 & 0 & \dots & 0 \\ 0 & \dots & 0 & 0 & 0 & 0 & 0 & -1 & 12 & 1 & 0 & \dots & 0 \\ \vdots & \dots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \dots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 509 & 1 \\ 0 & \dots & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 510 \end{bmatrix}_{1001 \times 1001}$$

$$B = \text{diag}(2, 3, \dots, 1002)_{1001 \times 1001}$$

We apply Algorithm shift-and-invert Arnoldi algorithm (Algorithm2) and Algorithm 3.

the results shown for Iterative=100, $m = 3$, $\tau = 600$, $\sigma = 2$

Algorithm(2) after Iterative=100 the residual norm is 510 i.e. it is not converge.but algorithm 3 after Iterative=100 the residual norm is .002 we see that algorithm 3 is better than algorithm 2.

the results shown for Iterative=200, $m = 4$, $\tau = 550$, $\sigma = 2$

Algorithm(2) after Iterative=200 the residual norm is 550 i.e. it is not converge.but algorithm 3 after Iterative=200 the residual norm is .003 we see that algorithm 3 is better than algorithm 2.

As the results show the new computational harmonic method projection algorithm (algorithm 3) works better than shift-and-invert method (algorithm 2) and it gives the results with high accuracy.

References

- [1] Y. Sadd, Numerical method for large eigenvalue problem, Manchester University press in Algorithm and architectures for advanced scientific computing 1992.
- [2] Y. Sadd, Iterative method for sparse linear system ,PWS Publishing Company, a division of international Thomson publishing Inc.,USA,1996.
- [3] G. Wu, A modified harmonic block Arnoldi Algorithm with adaptive shifts for large interior eigenproblems, Journal of computational and Applied Mathematics, 205 (2007) 343-365.
- [4] R. B. Morgan and M. Zeng, Harmonic projection method for large non-symmetric eigenvalue problem, Number Linear Algebra,Appl.5 (1998) 33-55.
- [5] G. H. Golub and C. F. Van Loan, Matrix computations second edition. The Johns Hopkins University Press, Baltimore, MD, 1989.
- [6] Z. Jia, The refined harmonic Arnoldi method and an implicitly restarted refine algorithm for computing interior eigepairs of large matrices, Applied numerical mathematics, 42 (2002) 489-512.
- [7] Z. Jia and Y. Zhang, A refined shift-and-invert Arnoldi algorithm for large un symmetric generalized eigenproblems, Computers and mathematics whit application 44 (2002) 1117-1127.

- [8] H. Saberi Najafi and H. Moosaei, A new restarting method in the harmonic projection algorithm for computing the eigenvalues of a nonsymmetric matrix, *Applied Mathematics and Computation*, (In press).
- [9] H. Saberi Najafi and H. Moosaei, The harmonic projection method for large non-symmetric generalized eigenproblem by shift-and-invert, submit to journal.

Received: November 6, 2007