Comparison Between FOM-Inverse and Weighted-FOM-Inverse and GS Method for Computing a Few Smallest (largest) Eigenvalues of Pair (A,B)

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Abstract

The generalized eigenvalue problem $AX = \lambda BX$ has special properties when (A, B) is a symmetric and positive definite pair.

We have recently developed three methods for computing a few smallest (largest) eigenvalues of a symmetric positive definite problem $AX = \lambda BX$ [2-3-4]. In this article we compared those methods by some numerical examples.

keywords: Generalized eigenvalue, Arnoldi, symmetric, positive definite, weighted FOM.

1. Introduction

Solving generalized eigenvalue problem, $AX = \lambda BX$, is one of the most important problems in numerical linear algebra. It's importance is because it is often used in a lot of engineering problems. In most of these cases we come across a symmetric positive definite generalized eigenvalue problem of the form $AX = \lambda BX$, where A and B are symmetric, and at least one of them is positive definite, for example in problems connected to mechanical vibration or analysis of structures.

There are several methods to solve generalized eigenvalue problem, $AX = \lambda BX$, but the number of computed eigenvalues by these methods might be less or more than expected. There are also methods which can lead us to the amount of results needed, like krylov subspace method, [5-12].

In this paper we compute P smallest (largest) eigenvalues which is very important in engineering problems, P is an arbitrary integer number. Our work is based on using inverse vector iteration method and solving the resulting system with the help of krylov subspace methods. After finding the smallest (largest) eigenvalue of pair (A, B), by using an appropriate deflation method on the new pair the next eigenvalue will be computed.

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2. Definition

2.1 If $X \in R^n$ and $\|X\|_2 = 1$, then the number $R(X) = \dfrac{X^T AX}{X^T BX}$ is called the generalized Rayleigh quotient. This quotient is well defined if and only if the matrix B is positive definite.

2.2 Let D be a diagonal matrix, i.e, $D = diag(d_1, d_2, \ldots, d_n)$. If U, V are two vectors of R^n. We define the D-scalar product of $(U \cdot V)_D = V^t DU$. This product is well defined if and only if matrix D is positive definite, i. e, $d_i > 0$, $i = 1,2,\ldots,n$. The norm associated with this inner product is the D-norm $\|\cdot\|_D$ and define by

$$\|U\|_D = \sqrt{(U.U)_D} = \sqrt{U^T DU} \quad \forall U \in R^n$$

3. Theorems

Theorem 3.1. The symmetric definite generalized eigenvalue problem has real eigenvalues and linearly independent eigenvectors.

Proof in [1]

Theorem 3.2. The generalized eigenvectors of pair (A, B) are B-orthonormal.

Proof in [1]

4.G-R Method

Theorem 4.1. Let $Y_i^{(m)}$ be an a eigenvector of symmetric tridiagonal matrix T_m associated with the eigenvalue $\lambda_i^{(m)}$, computed by Lanczos algorithm, and $U_i^{(m)}$, the Ritz approximate eigenvector, $U_i^{(m)} = V_m Y_i^{(m)}$ of pencil (A , B), then

i) $(A - \lambda_i^{(m)} B)U_i^{(m)} = \beta_m B v_{m+1} e_m^T Y_i^{(m)}$ and

$$\left\|(A - \lambda_i^{(m)} B)U_i^{(m)}\right\|_B = \beta_m \left\|B v_{m+1} e_m^T Y_i^{(m)}\right\|_B$$

$$\left\|(A - \lambda_i^{(m)} B)U_i^{(m)}\right\|_2 = \beta_m \left\|B v_{m+1} e_m^T Y_i^{(m)}\right\|_2$$

ii) If the matrix B be idempotent then :

$$\left\|(A - \lambda_i^{(m)} B)U_i^{(m)}\right\|_B = \left\|(A - \lambda_i^{(m)} B)U_i^{(m)}\right\|_2 = \beta_m \left|e_m^T Y_i^{(m)}\right|$$

Proof:

i) Since we have $AV_m = BV_m T_m + \beta_m B v_{m+1} e_m^T$

Therefore multiplying both sides of above relation by $Y_i^{(m)}$ can be written as,

$$AV_m Y_i^{(m)} = BV_m T_m Y_i^{(m)} + \beta_m B v_{m+1} e_m^T Y_i^{(m)}$$

So

$$(A - \lambda_i^m B)U_i^{(m)} = \beta_m B v_{m+1} e_m^T Y_i^{(m)}$$

ii) $\left\|(A - \lambda_i^{(m)} B)U_i^{(m)}\right\|_B^2 = \left\|\beta_m B v_{m+1} e_m^T Y_i^m\right\|_B^2 = (\beta_m Y_i^{T(m)} e_m v_{m+1}^T B^3 \beta_m v_{m+1} e_m^T Y_i^{(m)})$

Since B is idempotent so

$$= \beta_m^2 (Y_i^{T(m)} e_m V_{m+1}^T B V_{m+1} e_m^T Y_i^{(m)}$$
$$= \beta_m^2 (Y_i^{T(m)} e_m)(e_m^T Y_i^{(m)})$$
$$= \beta_m^2 (e_m^T Y_i^{(m)})^T (e_m^T Y_i^{(m)})$$
$$= \beta_m^2 \left| e_m^T Y_i^{(m)} \right|^2$$

And similarly

$$\left\| (A - \lambda_i^{(m)} B) U_i^{(m)} \right\|_2 = \beta_m^2 \left| e_m^T Y_i^{(m)} \right|^2$$

Finally

$$\left\| (A - \lambda_i^{(m)} B) U_i^{(m)} \right\|_2 = \left\| (A - \lambda_i^{(m)} B) U_i^{(m)} \right\|_B = \beta_m \left| e_m^T Y_i^{(m)} \right| \quad \square$$

Algorithm 1. Generalized Restarting process.(G-R) [2]

Choose an initial vector $\widetilde{V}_1$

Compute $V_1 = \dfrac{\widetilde{V}_1}{\left\| \widetilde{V}_1 \right\|_B}$

For k=1,2,…,m do

For s=1,2,…,m do

Run Lanczos algorithm for m step $(V_m^{(s)}, T_m^{(s)})$

Compute Lanczos Ritz value $\theta_i^{(s)}$ and generalized Ritz vector

Set $\gamma = \min \left\{ r_i^{(s)} = \left\| A\theta_i^{(s)} - \theta_i^{(s)} B Y_i^{(s)} \right\|_2 \right\}_{i=k}^{m}$

for p=k,k+1,…,m do

If $\gamma = Y_P^{(s)}$ then, set $V_1 = Y_P^{(s)}$ and B -normalized.

end if; end do; end do;

$Y_P^{(s)} \leftrightarrow Y_k^{(s)}$

$U_k = Y_k^{(s)}$

$V_1 = \sum_{j=1}^{k} U_j + \sum_{j=k+1}^{m} Y_j^{(s)}$ and B -normalized

End do.

Numerical test 1:
Let A and B are 1000×1000 matrices as:

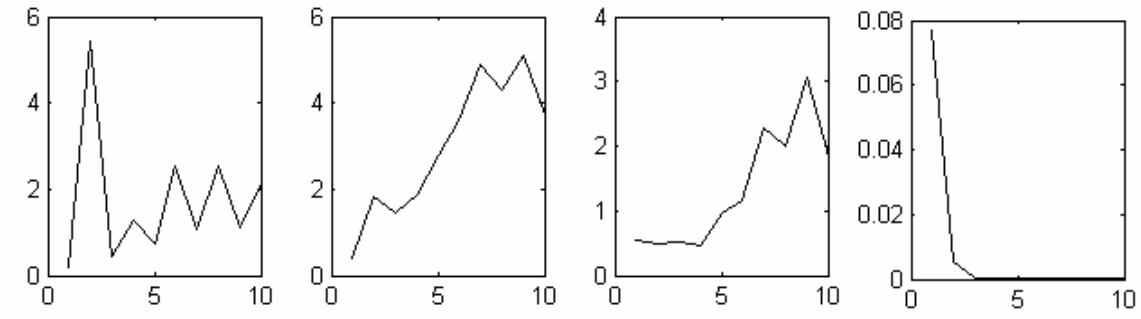
$$A=\begin{bmatrix}
1 & 1.2 & 0.42 & 0.8 & 0.3 & 0.8 & & & & & & & & & \\
1.2 & 2 & 1.2 & 0.42 & 0.8 & 0.3 & & & & & & & & & \\
0.42 & 1.2 & 3 & 1.2 & 0.42 & 0.8 & & & & & & & & & \\
0.8 & 0.42 & 1.2 & 4 & 1.2 & 0.42 & & & & & & & & & \\
0.3 & 0.8 & 0.42 & 1.2 & 5 & 1.2 & & & & & & & & & \\
0.8 & 0.3 & 0.8 & 0.42 & 1.2 & 6 & & & & & & & & & \\
 & 0.8 & 0.3 & 0.8 & 0.42 & 1.2 & & & & & & & & & \\
 & & 0.8 & 0.3 & 0.8 & 0.42 & & & & & & & & & \\
 & & & 0.8 & 0.3 & 0.8 & & & & & & & & & \\
 & & & & 0.8 & 0.3 & & & & & & & & & \\
 & & & & & 0.8 & & & & & & & & & \\
 & & & & & & 0.8 & & & & & & & & \\
 & & & & & & 0.3 & 0.8 & & & & & & & \\
 & & & & & & 0.8 & 0.3 & 0.8 & & & & & & \\
 & & & & & & 0.42 & 0.8 & 0.3 & & & & & & \\
 & & & & & & 1.2 & 0.42 & 0.8 & & & & & & \\
 & & & & & & 0.8 & 0.3 & 0.8 & 0.42 & 1.2 & 998 & 1.2 & 0.42 & \\
 & & & & & & & 0.8 & 0.3 & 0.8 & 0.42 & 1.2 & 999 & 1.2 & \\
 & & & & & & & & 0.8 & 0.3 & 0.8 & 0.42 & 1.2 & 1000
\end{bmatrix}_{1000\times1000}$$

$$B = Diag(2,3,\ldots,1000,1001)_{1000\times1000}$$

We apply algorithm 1 for m=4.The results are shown in Fig1, Fig2, Fig3, and Fig4

Fig 1

Showing the improvement of the first generalized eigenvalue (λ_1) in the first step of generalized



Restarting after a number of restarts

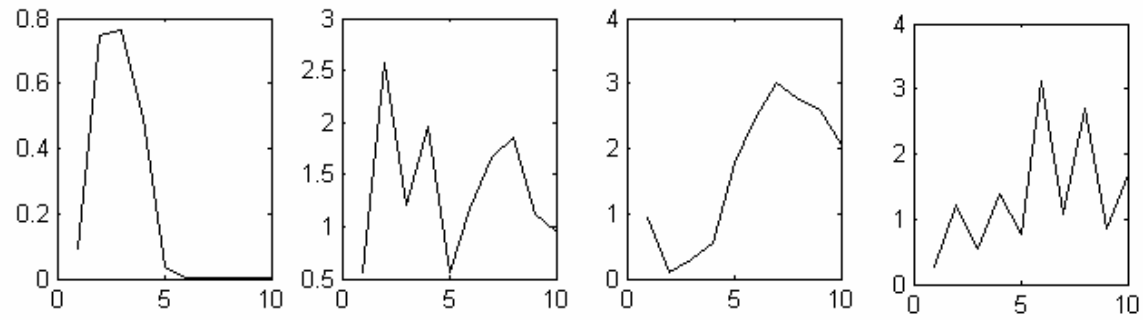


Fig 2

Showing the improvement of the fourth generalized eigenvalue (λ_4) in the second step of generalized restarting after a number of restarts

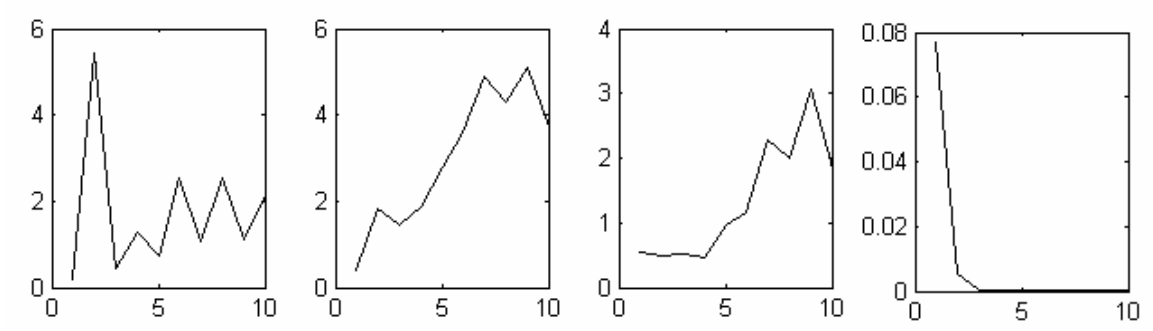


Fig 3

Showing the improvement of the third generalized eigenvalue ((λ_3)) in the third step of generalized restarting after a number of

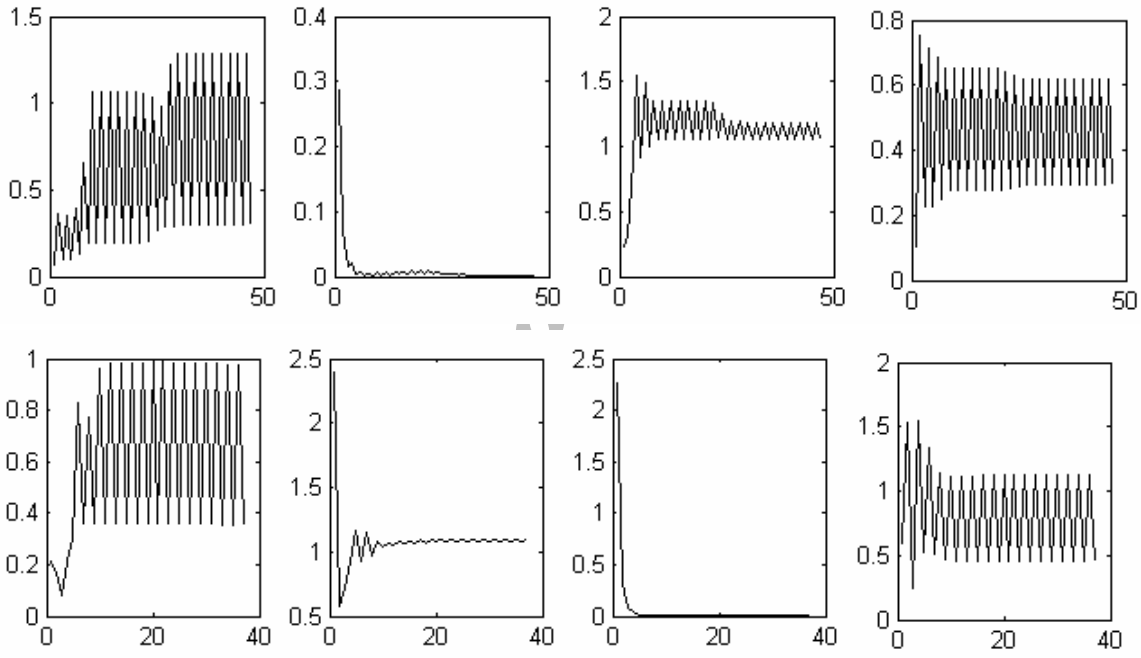
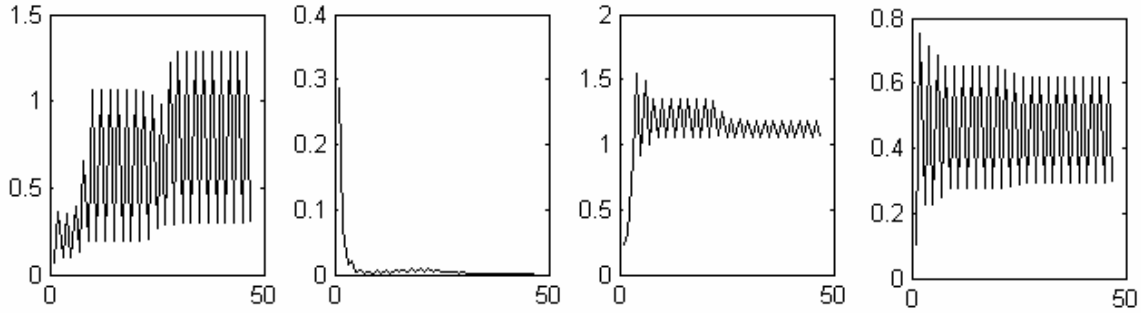


Fig 4

Showing the improvement of the second generalized eigenvalue ((λ_2)) in the fourth step of generalized restarting after a number of restarts.



$\|\ \|_B$				$\|\ \|_2$			
Step	**Iteration**	**Error**	**Time**	**Step**	**Iteration**	**Error**	**Time**
1	10	3.5439e-8	17.0288	1	10	1.38e-9	17.1634
2	10	4.88e-13	17.3324	2	10	1.7225e-14	16.7966
3	50	9.5053e-5	83.6560	3	37	9.3618e-5	62.0779
4	49	0.0001637	82.0542	4	47	0.0000157	78.6765
	119	2.5888e-4	200.0714		104	6.281e-5	174.7144

5. FOM- inverse Vector iteration method

Algorithm 2. FOM-inverse vector iteration method [3]

Input initial vector x_1 whit $\|x_1\| = 1$ and tolerance ε and parameter m .

$$\lambda_1 = \frac{x_1^T A x_1}{x_1^T B x_1}$$

$x_m = x_1$

For k=1, 2,…do

Compute $r_0 = Bx_k - Ax_m$

For z=1,2,… do

Compute $\beta = \|r_0\|_2$ and $v_1 = \frac{r_0}{\beta}$

Construct the orthonormal basis V_m by the Arnoldi process, starting with v_1

Solve $H_m Y_m = \beta e_1$, and set $x_m = x_0 + V_m Y_m$, $r_m = Bx_k - Ax_m$

If $\|r_m\| > \varepsilon$ then $x_0 = x_m$, $r_0 = r_m$ end {for} end {if}

$\tilde{x}_{k+1} = x_m$

$$\lambda_{k+1} = \frac{\tilde{x}_{k+1}^T A \tilde{x}_{k+1}}{\tilde{x}_{k+1}^T B \tilde{x}_{k+1}}$$

If $\frac{|\lambda_{k+1} - \lambda_k|}{\lambda_{k+1}} > \varepsilon$ then $x_{k+1} = \frac{\tilde{x}_{k+1}}{(\tilde{x}_{k+1} B \tilde{x}_{k+1})^{\frac{1}{2}}}$ end {for} end {if}

As algorithm 4 shows, there are 2 loops in this algorithm, one computes the eigenvector and is called outer iteration, the other solves the system of linear equation at each iteration, which is inner iteration. Numerical tests show that there are a significant relation between parameter m and inner-outer iterations.

Numerical test 2

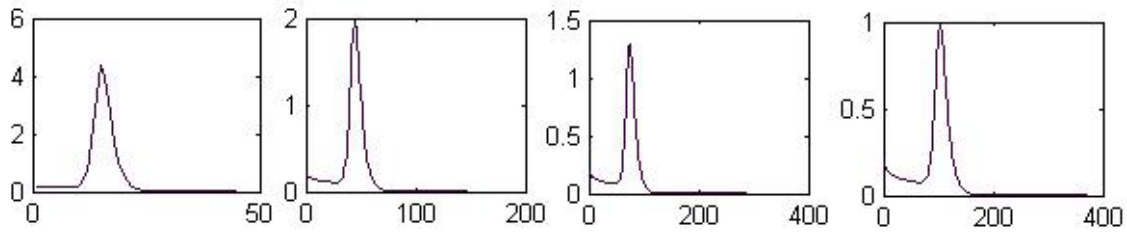
Let A and B are two 1000×1000 matrices used in numerical test 1. We apply algorithm 2 to find the smallest eigenvalue with initial vector v_1 and the stopping criterion is set as $\varepsilon \le 10^{-7}$ where $\varepsilon = \frac{|\lambda_{k+1} - \lambda_k|}{\lambda_{k+1}}$.

m	Inner iteration	Outer iteration	Total inner iteration	Tim
4	28	48	112	19.86
6	15	47	90	13.70
8	7	47	56	9.36
10	5	47	50	9.04
12	4	45	48	8.06

By applying algorithm 2 and deflation process [4] we find 4 smallest generalized eigenvalue of pair (A , B).

Fig 5

Showing number required outer-iterations for compute 4 smallest generalized eigenvalue of pair (A, B) with accuracy 10^{-7} .



6. Weighted FOM- inverse vector iteration method

Algorithm 3. Weighted FOM-inverse vector iteration method [4]

Input initial vector x_1 whit $\|x_1\| = 1$ and tolerance ε and parameter m .

$$\lambda_1 = \frac{x_1^T A x_1}{x_1^T B x_1}$$

$x_m = x_1$

For k=1,2,…do

Compute $r_0 = Bx_k - Ax_m$

For z=1,2,… do

Choose the vector d such as $\|d\|_2 = \sqrt{n}$ and set $D = diag(d)$

Compute $\widetilde{\beta} = \|r_0\|_D$ and $\widetilde{v}_1 = \frac{r_0}{\widetilde{\beta}}$

Construct the D-orthonormal basis $\widetilde{V}_m$ by the weighted Arnoldi process, starting with $\widetilde{v}_1$

Solve $\widetilde{H}_m Y_m = \widetilde{\beta}\, e_1$, and set $x_m = x_0 + \widetilde{V}_m Y_m$, $r_m = Bx_k - Ax_m$

If $\|r_m\|_2 > \varepsilon$ then $x_0 = x_m$, $r_0 = r_m$

end {for}

$\widetilde{x}_{k+1} = x_m$

$$\lambda_{k+1} = \frac{\widetilde{x}_{k+1}^T A \widetilde{x}_{k+1}}{\widetilde{x}_{k+1}^T B \widetilde{x}_{k+1}}$$

If $\frac{|\lambda_{k+1}-\lambda_k|}{\lambda_{k+1}} < \varepsilon$ then stop

Else $x_{k+1} = \frac{\widetilde{x}_{k+1}}{(\widetilde{x}_{k+1} B \widetilde{x}_{k+1})^{\frac{1}{2}}}$ end {for}

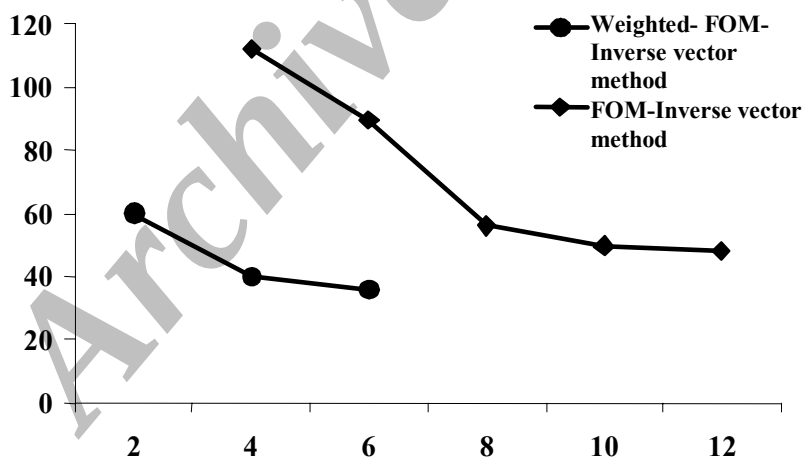
Numerical test 3 for G-R

Let A and B are two 1000×1000 matrices used in numerical test 1. We apply algorithm 3 to find the smallest eigenvalue with initial vector v_1 and the stopping criterion is set as $\varepsilon \le 10^{-7}$ where $\varepsilon = \frac{|\lambda_{k+1} - \lambda_k|}{\lambda_{k+1}}$.

m	Inner iteration	Outer iteration	Total inner iteration	Tim
2	30	29	60	53.04
4	10	28	40	18.87
6	6	27	36	12.49
8	6	27	48	24.11

Fig 6

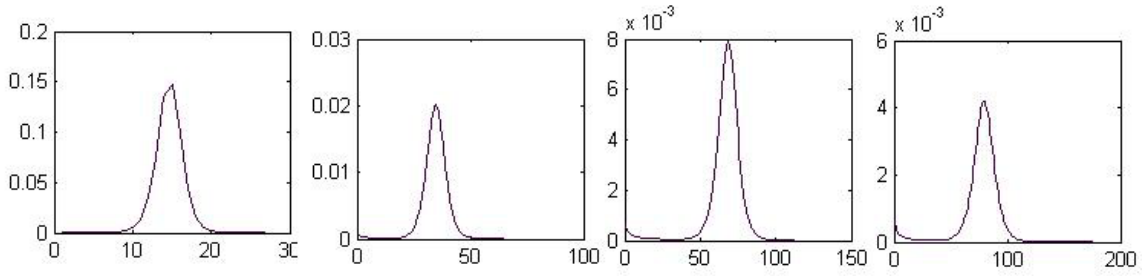
Comparing the total number of inner iterations needed to reach a desired accuracy for $m = 4,6,8,10,12$. By FOM inverse vector iteration method [7] and for $m = 2,4,6$ by W-FOM inverse vector iteration method which can be compared with the W-F-Inverse method.



By applying algorithm 3 and deflation process [4] we find 4 smallest generalized eigenvalue of pair (A , B).

Fig 7

Showing number required outer-iterations for compute 4 smallest generalized eigenvalue of pair (A, B) with accuracy 10^{-7}



7. Comparison between FOM-Inverse and Weighted-FOM- Inverse and GR methods

P	Iteration	Error	Time
GR method			
1	10	1.38e-9	17.1634
2	10	1.7225e-14	16.7966
3	37	9.3618e-5	62.0779
4	47	0.0000157	78.6765
	104	**6.281e-5**	**174.7144**
Fom-inverse vector iteration method			
1	45	1.41e-7	8.06
2	149	2.121e-7	72.67
3	289	1.134e-7	141.18
4	374	4.561e-7	178.114
	857	**2.1e-7**	**400.02**
WeightedFom-inverse vector iteration method			
1	27	1.91e-7	12.49
2	65	6.23e-7	46.09
3	113	3.123e-7	80.57
4	177	1.1e-7	125.67
	382	**3.3e-7**	**264.82**

8. Comments and conclusions.

1) As we know there are some methods for computing the rest of eigenvalues, for example, shift method but the advantage of this kind of deflation compared to the shift method is that for any $\delta_i > \lambda_{P+2}$ $(i = 1,2,\ldots,P)$ the method converges to $(P+1)^{th}$ eigenvalue but in the shift method if we don't use an appropriate shift value it might converge to another eigenvalue.

2) To compute the largest eigenvalue of (A , B), we just need to compute the smallest eigenvalue of (- A , B) and change the sign to obtain the largest eigenvalue of (A , B).

3) The vector d will be chosen as $d_i = \sqrt{n}\dfrac{|(r_0)_i|}{\|r_0\|_2}$. Such a choice favors the components of the residual which are far away from zero.

4) This algorithm has the advantage of letting us choose an appropriate m , so as to reach the necessary accuracy, meaning the smallest inner-outer iterations needed

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