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Restarted generalized Krylov subspace methods for solving large-scale polynomial eigenvalue problems

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Abstract In this paper, we introduce a generalized Krylov subspace $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$ based on a square matrix sequence $\{A_j\}$ and a vector sequence $\{u_j\}$. Next we present a generalized Arnoldi procedure for generating an orthonormal basis of $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$. By applying the projection and the refined technique, we derive a restarted generalized Arnoldi method and a restarted refined generalized Arnoldi method for solving a large-scale polynomial eigenvalue problem (PEP). These two methods are applied to solve the PEP directly. Hence they preserve essential structures and properties of the PEP. Furthermore,

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restarting reduces the storage requirements. Some theoretical results are presented. Numerical tests report the effectiveness of these methods.

Keywords Polynomial eigenvalue problem · Generalized Krylov subspace · Generalized Arnoldi procedure · Projection technique · Refined technique · Restarting

Mathematics Subject Classifications 65F10 · 65F15

1 Introduction

In this paper we will present generalized Krylov subspace methods for computing the eigenpairs of the polynomial eigenvalue problem (PEP) (see [4, 8, 14, 18, 28]).

$$\left(\lambda^n M_n + \lambda^{n-1} M_{n-1} + \cdots + M_0\right) x = 0, \tag{1.1}$$

where $M_0, M_1, \ldots, M_n \in \mathbb{R}^{N\times N}$, are real matrices and $x \in \mathbb{R}^N$ is the eigenvector corresponding to the eigenvalue λ.

Especially, when $n = 2$, the quadratic eigenvalue problem (QEP) is one of the most important problems that arises in many applications, such as finite element discretization in structural analysis [22] and the elastic deformation of anisotropic materials [21]. For a current review of numerical methods for QEP along with a broad discussion of application areas, see Tisseur and Meerbergen [27].

When $n = 3$, the cubic eigenvalue problem (CEP) also plays an important role in many applications [12], for example, a semiconductor quantum dot model with non-parabolic band structure described by the three-dimensional (3D) Schrödinger equation can result in a CEP with order up to 211400 from the finite difference approximation.

The classical approach in solving the PEP is to turn it into a linear eigenvalue problem. In the case of (1.1) this leads to the linearized generalized eigenvalue problem

$$\left(\lambda \begin{bmatrix} M_n & 0 & \cdots & 0 \\ 0 & I & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & I \end{bmatrix} - \begin{bmatrix} -M_{n-1} & -M_{n-2} & \cdots & -M_0 \\ I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & I & 0 \end{bmatrix}\right) \begin{bmatrix} \lambda^{n-1}x \\ \lambda^{n-2}x \\ \vdots \\ x \end{bmatrix} = 0, \tag{1.2}$$

or an equivalent eigenvalue problem

$$\begin{bmatrix} -M_n^{-1}M_{n-1} & -M_n^{-1}M_{n-2} & \cdots & -M_n^{-1}M_0 \\ I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & I & 0 \end{bmatrix} \begin{bmatrix} \lambda^{n-1}x \\ \lambda^{n-2}x \\ \vdots \\ x \end{bmatrix} = \lambda \begin{bmatrix} \lambda^{n-1}x \\ \lambda^{n-2}x \\ \vdots \\ x \end{bmatrix}, \tag{1.3}$$

where we assume throughout the paper that M_n is nonsingular.

If $(\lambda, [\lambda^{n-1}x^T, \lambda^{n-2}x^T, \cdots, x^T]^T)$ is an eigenpair of (1.2), then x is an eigenvector of (1.1) associated with the eigenvalue λ. When $n = 2$, the approach (1.2) allows us to determine eigenpairs numerically [6]. However it suffers some disadvantages such as solving the eigenvalue problem (1.2) of n times of the dimension of the original PEP, and more importantly, the loss of original structures of the PEP in the process of linearization.

For recent years, researchers have been studying for numerical methods [2, 7, 9–11, 13, 17, 26, 27] which can be applied to solve the large-scale QEP directly. In these methods, they do not transform the QEP to an equivalent linear form; instead, they project the QEP onto a properly chosen low-dimensional subspace to reduce to an QEP with lower order directly. The reduced QEP can then be solved by a standard dense matrix technique. The Jacobi-Davidson method [23, 24] is one of such methods. The method targets at one eigenvalue at one time with local convergence versus Krylov subspace methods in which a group of eigenvalues is approximated with global convergence. A direct Krylov-type subspace method with a generalized Arnoldi procedure is briefly described in [19]. A novel explicit non-equivalence deflation method [12] for solving the CEP with low-rank updates is developed and analyzed.

Recently, a second-order Arnoldi (SOAR for short) method using projection technique for finding a few eigenvalues, often those with the largest magnitude, and the corresponding eigenvectors of large-scale QEP is proposed in [3]. The remarkable feature in practice is that these methods are applied directly to solve the original problem, the essential structures of M_2, M_1, M_0 as well as the spectral properties are preserved promisingly.

Since both the expense and the storage of the SOAR algorithm increase as the method proceeds, restarting is generally necessary in practice. In this paper, we will propose two restarted methods for solving the CEP.

Throughout this paper, we use the following notations. I denotes the identity matrix, e_j denotes the j-th column of the identity matrix I, 0 denotes the zero vector or zero matrix. The dimensions of these vectors and matrices are conformed with dimensions used in the context. The superscript T denotes the transpose of a vector or a matrix. We denote 1-norm and 2-norm by $\|\cdot\|_1$ and $\|\cdot\|_2$, respectively, for a vector or a matrix.

The remainder of the paper is organized as follows. In Section 2, we introduce the generalized Krylov subspace $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$ and the generalized Arnoldi procedure for generating an orthonormal basis of the subspace. In Section 3, we present a restarted projection procedure and a restarted refined projection procedure for solving the CEP. Section 4 is devoted to some numerical tests. Some concluding remarks are given in Section 5.

2 The generalized Arnoldi procedure

In this section, we first define a generalized Krylov subspace of a square matrix sequence $\{A_j\}$ and a vector sequence $\{u_j\}$. Then we present a generalized

Arnoldi procedure for generating an orthonormal basis of the generalized Krylov subspace.

Definition 2.1 Let $A_0, A_1, \ldots, A_{n-1}$ be a square matrix sequence of order N, and $u_0, u_1, \ldots, u_{n-1}$ be an N-dimensional vector sequence with $u_{n-1} \neq 0$. Then the sequence

$$r_0, r_1, r_2, \ldots, r_{m-1}, \tag{2.1}$$

where

$$\begin{aligned} r_0 &= u_1, \\ r_1 &= u_2, \\ \vdots &= \vdots \\ r_{n-2} &= u_{n-1}, \\ r_{n-1} &= A_{n-1}u_{n-1} + A_{n-2}u_{n-2} + \cdots + A_0 u_0, \\ r_j &= A_{n-1}r_{j-1} + A_{n-2}r_{j-2} + \cdots + A_0 r_{j-n}, \quad for \quad j \geqslant n, \end{aligned}$$

is called a generalized Krylov sequence based on $\{A_j\}$ and $\{u_j\}$. The space

$$\mathcal{G}_m(\mathbf{A}; \mathbf{u}) = \text{span}\{r_{n-2}, r_{n-1}, \ldots, r_{n+m-3}\},$$

is called an m-th generalized Krylov subspace.

If one applies a Krylov subspace technique to (1.3), then an associated Krylov subspace would naturally be

$$\mathcal{K}_m(F; v_1) = \text{span}\left\{v_1, Fv_1, F^2v_1, \cdots, F^{m-1}v_1\right\}, \tag{2.2}$$

where v_1 is an initial vector of length $N \times n$, and

$$F = \begin{bmatrix} -M_n^{-1}M_{n-1} & -M_n^{-1}M_{n-2} & \cdots & -M_n^{-1}M_0 \\ I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & I & 0 \end{bmatrix}.$$

Let $A_{n-1} = -M_n^{-1}M_{n-1}$, $A_{n-2} = -M_n^{-1}M_{n-2}$, $\cdots$, $A_0 = -M_n^{-1}M_0$ and $v_1 = \left[u_{n-1}^T, u_{n-2}^T, \ldots, u_0^T\right]^T$, then it immediately derives that the generalized Krylov vectors $\{r_j\}$ of length N defined in (2.1) and the standard Krylov vectors $\{F^j v_1\}$ of length $N \times n$ defined in (2.2) is related as the following form

$$\begin{bmatrix} r_j \\ r_{j-1} \\ \vdots \\ r_{j-n+1} \end{bmatrix} = F^{j-n+2}v_1, \quad for \quad j \geqslant n-1. \tag{2.3}$$

Equation 2.3 indicates that the subspace $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$ of $\mathbb{R}^N$ should be able to provide sufficient information to let us directly work with the PEP, instead of using the subspace $\mathcal{K}_m(F; v_1)$ for the linearized eigenvalue problem (1.3).

The following procedure constructs the vectors $q_1^{(n-1)}, q_2^{(n-1)}, \cdots, q_m^{(n-1)}$ such that $\left\{q_1^{(n-1)}, q_2^{(n-1)}, \cdots, q_m^{(n-1)}\right\}$ is an orthonormal basis of the subspace

$\mathcal{G}_m(\mathbf{A}; \mathbf{u})$. We call it a GAR (Generalized ARnoldi) procedure. The algorithm is described as follows.

Algorithm 2.1 GAR procedure

1. $\beta = \|u_{n-1}\|_2$
2. $$\begin{bmatrix} q_1^{(n-1)} \\ q_1^{(n-2)} \\ \vdots \\ q_1^{(0)} \end{bmatrix} = \frac{1}{\beta} \begin{bmatrix} u_{n-1} \\ u_{n-2} \\ \vdots \\ u_0 \end{bmatrix}$$
3. for $j = 1, 2, \cdots, m$
4. $$\begin{bmatrix} q_{j+1}^{(n-1)} \\ q_{j+1}^{(n-2)} \\ \vdots \\ q_{j+1}^{(0)} \end{bmatrix} = \begin{bmatrix} A_{n-1} & A_{n-2} & \cdots & A_0 \\ I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & I & 0 \end{bmatrix} \begin{bmatrix} q_j^{(n-1)} \\ q_j^{(n-2)} \\ \vdots \\ q_j^{(0)} \end{bmatrix}$$
5. for $i = 1, 2, \cdots, j$
6. $h_{i,j} = (q_i^{(n-1)})^T q_{j+1}^{(n-1)}$
7. $$\begin{bmatrix} q_{j+1}^{(n-1)} \\ q_{j+1}^{(n-2)} \\ \vdots \\ q_{j+1}^{(0)} \end{bmatrix} = \begin{bmatrix} q_{j+1}^{(n-1)} \\ q_{j+1}^{(n-2)} \\ \vdots \\ q_{j+1}^{(0)} \end{bmatrix} - h_{i,j} \begin{bmatrix} q_i^{(n-1)} \\ q_i^{(n-2)} \\ \vdots \\ q_i^{(0)} \end{bmatrix}$$
8. end for
9. $h_{j+1,j} = \|q_{j+1}^{(n-1)}\|_2$
10. if $h_{j+1,j} = 0$, then stop
11. $$\begin{bmatrix} q_{j+1}^{(n-1)} \\ q_{j+1}^{(n-2)} \\ \vdots \\ q_{j+1}^{(0)} \end{bmatrix} = \frac{1}{h_{j+1,j}} \begin{bmatrix} q_{j+1}^{(n-1)} \\ q_{j+1}^{(n-2)} \\ \vdots \\ q_{j+1}^{(0)} \end{bmatrix}$$
12. end for

Let $\widetilde{H}_m$ denote the $(m+1) \times m$ upper Hessenberg matrix whose nonzero entries $h_{i,j}, i = 1, \cdots, m+1$ and $j = 1, \cdots, m$ are defined by Algorithm 2.1. H_m is the $m \times m$ matrix obtained from $\widetilde{H}_m$ by deleting the last row.

From the GAR procedure, we can deduce the following relations:

$$\sum_{i=0}^{n-1} A_i Q_m^{(i)} = Q_m^{(n-1)} H_m + q_{m+1}^{(n-1)} e_m^T h_{m+1,m}, \tag{2.4}$$

$$Q_m^{(j)} = Q_m^{(j-1)} H_m + q_{m+1}^{(j-1)} e_m^T h_{m+1,m}, \quad for \quad 1 \leqslant j \leqslant n-1. \tag{2.5}$$

With $\widetilde{H}_m$, (2.4) and (2.5) can be rewritten in the compact form

$$\begin{bmatrix} A_{n-1} & A_{n-2} & \cdots & A_0 \\ I & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & I & 0 \end{bmatrix} \begin{bmatrix} Q_m^{(n-1)} \\ Q_m^{(n-2)} \\ \vdots \\ Q_m^{(0)} \end{bmatrix} = \begin{bmatrix} Q_{m+1}^{(n-1)} \\ Q_{m+1}^{(n-2)} \\ \vdots \\ Q_{m+1}^{(0)} \end{bmatrix} \widetilde{H}_m. \tag{2.6}$$

This relation assembles the similarity between the GAR procedure and the well-known Arnoldi procedure [1].

Now, we prove that the vector sequence $\{q_1^{(n-1)}, q_2^{(n-1)}, \ldots, q_m^{(n-1)}\}$ indeed is an orthonormal basis of the generalized Krylov subspace $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$. In [3], the following lemma is given.

Lemma 2.2 *Let A be an arbitrary $n \times n$ matrix. Let $V_{m+1} = [V_m \;\; v_{m+1}]$ be an $n \times (m+1)$ rectangular matrix that satisfies*

$$A V_m = V_{m+1} \widetilde{H}_m$$

for an $(m+1) \times m$ upper Hessenberg matrix $\widetilde{H}_m$. Then there is an upper triangular matrix R_m such that

$$V_m R_m = \left[\, v_1 \; A v_1 \; \cdots \; A^{m-1} v_1 \, \right].$$

Furthermore, if the first $m-1$ subdiagonal elements of $\widetilde{H}_m$ are nonzero, then R_m is nonsingular and

$$\operatorname{span}\{V_m\} = \mathcal{K}_m(A, v_1).$$

We now prove that Algorithm 2.1 generates an orthonormal basis of the generalized Krylov subspace $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$.

Theorem 2.3 *If $h_{j+1,j} \neq 0$ for $j \geqslant 1$ in Algorithm* 2.1. *Then the vector sequence $\{q_1^{(n-1)}, q_2^{(n-1)}, \ldots, q_j^{(n-1)}\}$ forms an orthonormal basis of the generalized Krylov subspace $\mathcal{G}_j(\mathbf{A}; \mathbf{u})$, i.e.,*

$$\operatorname{span}\left\{ Q_j^{(n-1)} \right\} = \mathcal{G}_j(\mathbf{A}; \mathbf{u}) \quad for \quad j \geqslant 1 \tag{2.7}$$

and $\left(q_i^{(n-1)}\right)^T q_k^{(n-1)} = 0$ if $i \neq k$ and $\left(q_i^{(n-1)}\right)^T q_i^{(n-1)} = 1$, for $i = 1, 2, \cdots, j$.

Proof Equation 2.7 is established by the following sequence of equalities:

$$
\begin{aligned}
\mathcal{G}_j(\mathbf{A};\mathbf{u}) &= \operatorname{span}\{r_{n-2}, r_{n-1}, \cdots, r_{n+j-3}\} \\
&= \operatorname{span}\left\{ \begin{bmatrix} I & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} u_{n-1} & r_{n-1} & \cdots & r_{n+j-3} \\ u_{n-2} & r_{n-2} & \cdots & r_{n+j-4} \\ \vdots & \vdots & \cdots & \vdots \\ u_0 & r_0 & \cdots & r_{j-2} \end{bmatrix} \right\} \\
&= \operatorname{span}\left\{ \begin{bmatrix} I & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} v_1 & Fv_1 & \cdots & F^{j-1}v_1 \end{bmatrix} \right\} \quad \text{by (2.3)} \\
&= \operatorname{span}\left\{ \begin{bmatrix} I & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} Q_j^{(n-1)} \\ Q_j^{(n-2)} \\ \vdots \\ Q_j^{(0)} \end{bmatrix} R_j \right\} \quad \text{by (2.6) and Lemma 2.2} \\
&= \operatorname{span}\left\{ \begin{bmatrix} I & 0 & \cdots & 0 \end{bmatrix} \begin{bmatrix} Q_j^{(n-1)} \\ Q_j^{(n-2)} \\ \vdots \\ Q_j^{(0)} \end{bmatrix} \right\} \\
&= \operatorname{span}\{Q_j^{(n-1)}\}.
\end{aligned}
$$

Algorithm 2.2 GAR procedure with memory saving (n=3)

```
1.  q_1 = u_2/‖u_2‖_2
2.  p_1 = u_1/‖u_2‖_2
3.  f = u_0/‖u_2‖_2
4.  for j = 1, ··· , m
5.      q_{j+1} = A_2 q_j + A_1 p_j + A_0 f
6.      p_{j+1} = q_j
7.      for i = 1, 2, ··· , j
8.          h_{i,j} = q_i^T q_{j+1}
9.          q_{j+1} = q_{j+1} − h_{i,j} q_i
10.         p_{j+1} = p_{j+1} − h_{i,j} p_i
11.     end for
12.     h_{j+1,j} = ‖q_{j+1}‖_2
13.     if h_{j+1,j} = 0, then stop
14.     q_{j+1} = q_{j+1}/h_{j+1,j}
15.     p_{j+1} = p_{j+1}/h_{j+1,j}
16.     f = (P(:, 1 : j) − u_0 H(1, 1 : j)) H(2 : j + 1, 1 : j)^{−1} e_j
17. end for
```

Finally, the orthogonality of the basis vectors $\{q_1^{(n-1)}, q_2^{(n-1)}, \ldots, q_j^{(n-1)}\}$ is directly obtained from the orthogonalization inner for-loop (lines 5–8) and normalization step at line 11 of the GAR procedure. □

In the rest of this section, we derive a new version of the GAR procedure by using the relations in Algorithm 2.1. In view of (2.5), for $Q_{m+1}^{(0)}$ partitioned as $Q_{m+1}^{(0)} = \left[q_1^{(0)},\ \hat{Q}^{(0)}\right]$, we can write

$$Q_m^{(1)} = Q_{m+1}^{(0)} \widetilde{H}_m = q_1^{(0)} \cdot \widetilde{H}_m(1,:) + \hat{Q}^{(0)} \cdot \widetilde{H}_m(2 : m+1,:).$$

So we can compute the vector $q_{j+1}^{(0)}$ from $Q_j^{(1)}$ and $H(1 : j+1, 1 : j)$. The new procedure reduces memory requirement by almost $1/n$.

For the rest of this paper, we are concerned only with $n = 3$.

3 Two projection methods for the CEP

In this section, we first apply the concept of the generalized Krylov subspace and its orthonormal basis generated by the GAR procedure to develop a projection technique to solve the CEP

$$\left(\lambda^3 M + \lambda^2 D + \lambda K + W\right) x = 0, \tag{3.1}$$

where $M,\ D,\ K,\ W \in \mathbb{R}^{N\times N}$, are real matrices and $x \in \mathbb{R}^N$ is the eigenvector corresponding to the eigenvalue λ.

We follow the orthogonal Rayleigh-Ritz approximation procedure [15, 16] to derive a method which approximates a large-scale CEP by a small-size CEP.

Following the standard derivation, to apply Rayleigh-Ritz approximation technique based on the subspace $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$ with $A_2 = -M^{-1}D$, $A_1 = -M^{-1}K$ and $A_0 = -M^{-1}W$, we seek an approximate eigenpair (θ, z), where $\theta \in \mathbb{C}$ and $z \in \mathcal{G}_m(\mathbf{A}; \mathbf{u})$, by imposing the following orthogonal condition, also called the Galerkin condition,

$$\left(\theta^3 M + \theta^2 D + \theta K + W\right) z \quad \perp \quad \mathcal{G}_m(\mathbf{A}; \mathbf{u}),$$

or equivalently,

$$v^T \left(\theta^3 M + \theta^2 D + \theta K + W\right) z = 0 \quad \text{for all} \quad v \in \mathcal{G}_m(\mathbf{A}; \mathbf{u}). \tag{3.2}$$

Since $z \in \mathcal{G}_m(\mathbf{A}; \mathbf{u})$, it can be written as

$$z = Q_m g, \tag{3.3}$$

where the $N \times m$ matrix Q_m is an orthonormal basis of $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$ generated by the GAR procedure (Algorithm 2.2), and g is an m-dimensional vector. By (3.2) and (3.3), it yields that θ and g must satisfy the reduced CEP:

$$\left(\theta^3 M_m + \theta^2 D_m + \theta K_m + W_m\right) g = 0 \tag{3.4}$$

with

$$M_m = Q_m^T M Q_m, \quad D_m = Q_m^T D Q_m, \quad K_m = Q_m^T K Q_m, \quad W_m = Q_m^T W Q_m. \tag{3.5}$$

The eigenpair (θ, g) of (3.4) defines the Ritz pair (θ, z). The Ritz pair is an approximate eigenpair of the CEP (3.1). The accuracy of the approximate eigenpair (θ, z) can be assessed by the norm of the residual vector $(\theta^3 M + \theta^2 D + \theta K + W)z$.

We note that by explicitly formulating the matrices M_m, D_m, K_m and W_m, essential structures of M, D, K and W are preserved. For example, if M is symmetric positive definite, so is M_m. As a result, essential spectral properties of the CEP will be preserved.

We define the following structure of method for solving the CEP (3.1).

Algorithm 3.1 The GAR method for solving the CEP

1. Choose three starting vectors u_0, u_1 and u_2.
2. Run GAR procedure (Algorithm 2.2) with $A_2 = -M^{-1}D$, $A_1 = -M^{-1}K$ and $A_0 = -M^{-1}W$ to generate an $N \times m$ orthogonal matrix Q_m whose columns span an orthonormal basis of $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$.
3. Compute M_m, D_m, K_m and W_m as defined in (3.5).
4. Solve the reduced CEP (3.4) for (θ, g) and obtain the Ritz pairs (θ, z), where $z = Q_m g / \| Q_m g \|_2$.
5. Test the accuracy of Ritz pairs (θ, z) as approximate eigenvalues and eigenvectors of the CEP (3.1) by the relative norms of residual vectors:

$$\frac{\|(\theta^3 M + \theta^2 D + \theta K + W)z\|_2}{|\theta|^3 \|M\|_1 + |\theta|^2 \|D\|_1 + |\theta| \|K\|_1 + \|W\|_1}. \tag{3.6}$$

About Algorithm 3.1, a few remarks, which were given in [3], are in order:

At step 2, the matrix-vector product operations $-M^{-1}Du$, $-M^{-1}Ku$ and $-M^{-1}Wu$ for an arbitrary vector u must be provided to run the GAR procedure (Algorithm 3.1). A factorized form of M, such as the LU factorization [5, 6], should be made available outside of the first for loop of Algorithm 3.1 for computational efficiency.

At step 4, to solve the small-size CEP (3.4), we transform it to a generalized eigenvalue problem in the form of (1.2), and then use a dense matrix method, such as the QZ algorithm [5, 6], to find all eigenvalues and eigenvectors (θ, g) of the small-size CEP.

At step 5, we use the relative residual norms (3.6) as the accuracy assessment to indicate the backward errors of the approximate eigenpairs (θ, z). The discussion of forward errors of approximate eigenvalues and eigenvectors is beyond the scope of this paper, and readers are referred to [25, 27].

A difficulty with the GAR method is that it becomes increasingly expensive as the number m increases. To remedy this difficulty, we can use the algorithm iteratively, i.e., we can restart the algorithm every m steps, where m is some fixed integer parameter. After obtaining k desired Ritz pairs $(\theta_i, z_i), i = 1, 2, \cdots, k$ for CEP (3.1), we can view $\left(\theta_i, (\theta_i^2 z_i^T, \theta_i z_i^T, z_i^T)^T\right)$ as the approximate eigenpairs of the linear eigenvalue problem (1.3) since the CEP (3.1) is equivalent to the linear eigenvalue problem (1.3) with $n = 3$. For the linear eigenvalue problem, Saad [20] suggested that the new starting vector in restarted methods should be set to a weighted combination of the desired approximate vectors, and the desired approximate vectors be weighted by the corresponding relative residual norms. In the restarted GAR, we generated the new starting vector by this technique.

This restarted version of GAR denoted by GAR(m) is described as follows.

Algorithm 3.2 GAR(m): Restarted GAR method for solving the CEP

1. Choose m, the maximum size of the subspace, and k, the desired number of approximate eigenpairs. Choose three starting vectors u_0, u_1 and u_2.
2. Run GAR procedure (Algorithm 2.2) with $A_2 = -M^{-1}D$, $A_1 = -M^{-1}K$ and $A_0 = -M^{-1}W$ to generate an $N \times m$ orthogonal matrix Q_m whose columns span an orthonormal basis of $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$.
3. Compute M_m, D_m, K_m and W_m as defined in (3.5).
4. Solve the reduced CEP (3.4) for (θ_i, g_i) and obtain the Ritz pairs (θ_i, z_i), where $z_i = Q_m g_i / \|Q_m g_i\|_2$ with $i = 1, 2, \cdots, k$.
5. Test the accuracy of Ritz pairs (θ_i, z_i) as approximate eigenvalues and eigenvectors of the CEP (3.1) by the relative norms of residual vectors:

$$\alpha_i := \frac{\|(\theta_i^3 M + \theta_i^2 D + \theta_i K + W) z_i\|_2}{|\theta_i|^3 \|M\|_1 + |\theta_i|^2 \|D\|_1 + |\theta_i| \|K\|_1 + \|W\|_1}.$$

If it is satisfied then stop, otherwise compute new starting vectors u_0, u_1 and u_2 by

$$\begin{bmatrix} u_2 \\ u_1 \\ u_0 \end{bmatrix} = \sum_{i=1}^{k} \alpha_i \begin{bmatrix} \theta_i^2 z_i \\ \theta_i z_i \\ z_i \end{bmatrix}$$

and go to 2.

Remark 3.1 This approach has two advantages over traditional approaches. The number of sought eigenvalues is pre-specified. The storage requirements is fixed instead of allowing them to become arbitrarily large.

For the linear eigenvalue problem, it has been revealed that the standard projection methods may converge very slowly and even may fail to converge. In order to correct this problem, Jia [15, 16] proposed the refined skill. In the rest of this section, we extend his idea to obtain the restarted refined generalized Arnoldi method for solving the CEP (3.1).

After obtaining k desired Ritz values $\theta_i, i = 1, 2, \cdots, k$ for CEP (3.1), now we seek k unit length vectors $\hat{z}_i = \mathcal{Q}_m \hat{g}_i$, which are called refined vectors and satisfy

$$\begin{aligned}
&\left\| \left(\theta_i^3 M + \theta_i^2 D + \theta_i K + W\right) \hat{z}_i \right\|_2 \\
&= \min_{z \in \mathcal{G}_m(\mathbf{A};\mathbf{u}), \|z\|_2 = 1} \left\| \left(\theta_i^3 M + \theta_i^2 D + \theta_i K + W\right) z \right\|_2 \\
&= \min_{g \in \mathbb{C}^n, \|g\|_2 = 1} \left\| \left(\theta_i^3 M + \theta_i^2 D + \theta_i K + W\right) \mathcal{Q}_m g \right\|_2 \\
&= \min_{g \in \mathbb{C}^n, \|g\|_2 = 1} \left\| \left(\theta_i^3 M \mathcal{Q}_m + \theta_i^2 D \mathcal{Q}_m + \theta_i K \mathcal{Q}_m + W \mathcal{Q}_m\right) g \right\|_2 .
\end{aligned}$$

It is easy to see that $\hat{g}_i$ is nothing but the right singular vector associated with the smallest singular value of the $N \times m$ matrix

$$T_i := \theta_i^3 M \mathcal{Q}_m + \theta_i^2 D \mathcal{Q}_m + \theta_i K \mathcal{Q}_m + W \mathcal{Q}_m. \tag{3.7}$$

This approximate eigenpair $(\theta_i, \hat{z}_i)$, called the refined Ritz pair, is better than the Ritz pair (θ_i, z_i) due to its minimal property. Thus, we can propose the restarted refined version of GAR, which is denoted by RGAR(m) and described as follows.

Algorithm 3.3 RGAR(m): Restarted refined GAR method for solving the CEP

1. Choose m, the maximum size of the subspace, and k, the desired number of approximate eigenpairs. Choose three starting vectors u_0, u_1 and u_2.
2. Run GAR procedure (Algorithm 2.2) with $A_2 = -M^{-1}D$, $A_1 = -M^{-1}K$ and $A_0 = -M^{-1}W$ to generate an $N \times m$ orthogonal matrix $\mathcal{Q}_m$ whose columns span an orthonormal basis of $\mathcal{G}_m(\mathbf{A}; \mathbf{u})$.
3. Compute M_m, D_m, K_m and W_m as defined in (3.5).
4. Solve the reduced CEP (3.4) and obtain the desired Ritz values θ_i, $i = 1, \cdots, k$. Compute the right singular vector $\hat{g}_i$ associated with the smallest singular value of the matrix T_i defined by (3.7), $i = 1, 2, \cdots, k$ and obtain k desired approximate eigenpairs $(\theta_i, \hat{z}_i = \mathcal{Q}_m \hat{g}_i)$.
5. Test the accuracy of refined Ritz pairs $(\theta_i, \hat{z}_i)$ as approximate eigenvalues and eigenvectors of the CEP (3.1) by the relative norms of residual vectors:

$$\alpha_i := \frac{\left\| \left(\theta_i^3 M + \theta_i^2 D + \theta_i K + W\right) \hat{z}_i \right\|_2}{|\theta_i|^3 \|M\|_1 + |\theta_i|^2 \|D\|_1 + |\theta_i| \|K\|_1 + \|W\|_1}.$$

   If it is satisfied then stop, otherwise compute new starting vectors u_0, u_1 and u_2 by

$$\begin{bmatrix} u_2 \\ u_1 \\ u_0 \end{bmatrix} = \sum_{i=1}^{k} \alpha_i \begin{bmatrix} \theta_i^2 \hat{z}_i \\ \theta_i \hat{z}_i \\ \hat{z}_i \end{bmatrix}$$

   and go to 2.

Remark 3.2 At step 4 in Algorithm 3.3, to generate $T_i, i = 1, 2, \cdots, k$, we need to compute $M\mathcal{Q}_m$, $D\mathcal{Q}_m$, $K\mathcal{Q}_m$ and $W\mathcal{Q}_m$ only one time. However, we note that $M\mathcal{Q}_m$, $D\mathcal{Q}_m$, $K\mathcal{Q}_m$ and $W\mathcal{Q}_m$ have been already obtained when M_m, D_m, K_m and W_m are computed at Step 3. Thus, we should save $M\mathcal{Q}_m$, $D\mathcal{Q}_m$, $K\mathcal{Q}_m$ and $W\mathcal{Q}_m$ at Step 3 in order to save the expense. In order to obtain the right singular vector $\hat{g}_i$ associated with the smallest singular value of the matrix T_i, we can compute the eigenvector associated with the smallest eigenvalue of $T_i^T T_i$.

4 Numerical tests

In this section, we present some numerical examples to illustrate the effectiveness of the GAR(m) method and the RGAR(m) method for solving the CEP (3.1).

In the following examples, the starting vector u_2 of the GAR(m) method and RGAR(m) method is chosen as a vector with all components equal to 1 and $u_0 = u_1 = 0$. The so-called exact eigenvalues of the CEP are computed by the dense method, namely, the QZ method for computing all eigenvalues and eigenvectors of the generalized eigenvalue problem (1.2) with $n = 3$. All numerical experiments are performed on an AMD 1.4 GHz PC with main memory 512 MB. The stop criterion is

$$\max_{1\leqslant i\leqslant k}\left(\frac{\left\|\left(\theta_i^3 M+\theta_i^2 D+\theta_i K+W\right) z_i\right\|_2}{|\theta_i|^3\|M\|_1+|\theta_i|^2\|D\|_1+|\theta_i|\|K\|_1+\|W\|_1}\right)\leqslant 10^{-8},$$

where k is the number of the desired eigenvalues.

Example 1 For the first test, we compare the convergence result of GAR(10) method and RGAR(10) method. Let M, D, K and W be 200×200 random nonsymmetric matrices. Elements of these matrices are chosen from a normal distribution with mean zero, variance one and standard deviation one. $m = 10$ and $k = 2$. The left plot of Fig. 1 shows the relative residual norms of the first largest magnitude approximate eigenpair and the right plot of Fig. 1 shows the relative residual norms of the second largest magnitude approximate eigenpair.

From Fig. 1, we know the cycle number of RGAR(10) is 4 and the cycle number of GAR(10) is 13, which shows that RGAR(10) converges faster than GAR(10) for this example.

Example 2 In this example, $M = 5 * I$, $D = 3 * \text{tridiag}(-1, 3, -1)$ and $K = W$ comes from the Matlab test matrix *bwm*200. These matrices are 200×200. We only compute the largest magnitude eigenvalue, i.e., $k = 1$. The plot of Fig. 2 shows the relative residual norms of the largest magnitude approximate

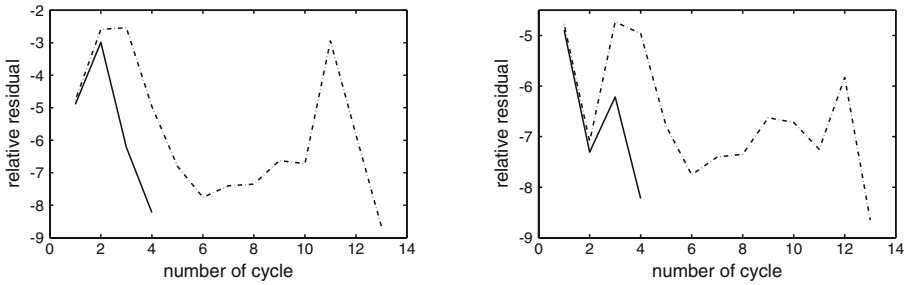

Fig. 1 Convergence plots of GAR(10) (*dash-dot line*) and RGAR(10) (*solid line*)

eigenpair with $m = 20$. The cycle number and cputime for RGAR(20) are 82 times and 12.23 s, respectively. However, the cycle number and cputime for GAR(20) are 98 times and 14.36 s, respectively.

Example 3 For the third experiment, we use some structural engineering matrices from the Harwell-Boeing collection to compare GAR(n) method and RGAR(n) method. These matrices all represent dynamic analysis in structural engineering. $M = 5 * I$, $D = 3 * \text{tridiag}(-1, 3, -1)$. The data of matrices K and W are extracted from bcsstm06 and bcsstk06, respectively. These matrices are 420×420. $m = 10$ and $k = 2$. The left plot of Fig. 2 shows the relative residual norms of the first largest magnitude approximate eigenpair and the right plot of Fig. 2 shows the relative residual norms of the second largest magnitude approximate eigenpair.

From Fig. 2, we know the cycle number of RGAR(10) is 155 and the cycle number of GAR(10) is 165, which shows that RGAR(10) converges faster than RGAR(10) for this example.

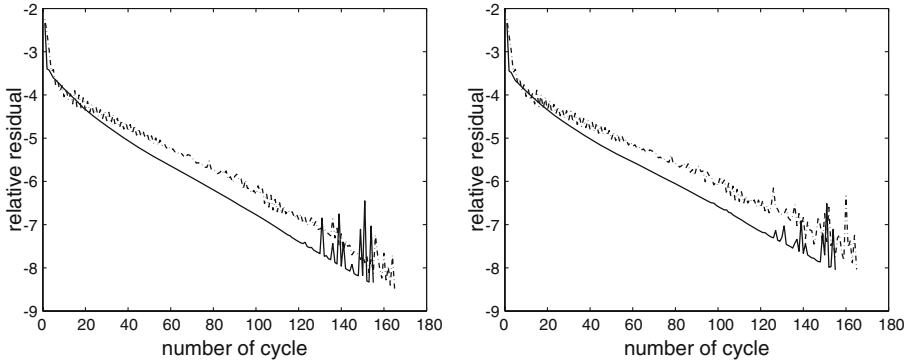

Fig. 2 Convergence plots of GAR(10) (*dash-dot line*) and RGAR(10) (*solid line*)

Example 4 For the last example we compare the performances of the SOAR method [3] and the restarted refined GAR method for solving the QEP. Let M, D and K be 200×200 random nonsymmetric matrices. Elements of these matrices are chosen from a normal distribution with mean zero, variance one and standard deviation one. $m = 10$ and $k = 2$. The so-called *exact* eigenvalues of the QEP are computed by the standard dense method, namely, the QZ method for computing all eigenvalues and eigenvectors of the generalized eigenvalue problem (1.3) for $n = 2$. The eigenvalues with the largest magnitude computed by the standard dense matrix method, and by RGAR(10) and SOAR methods are

$$\begin{aligned}\lambda_1 &= -25.34119207711575 \text{ (“Exact”)}\\ \lambda_1^R &= \underline{-25.34119207}014336 \text{ (RGAR(10))}\\ \lambda_1^S &= \underline{-25.3}7243332108736 \text{ (SOAR)}\end{aligned}$$

and

$$\begin{aligned}\lambda_2 &= 5.12792486919446 + 7.60620966180964i \text{ (“Exact”)}\\ \lambda_2^R &= \underline{5.12792}528188211 + \underline{7.60620}904785062i \text{ (RGAR(10))}\\ \lambda_2^S &= \underline{5.1}9745302967508 + \underline{7}.75745301359064i \text{ (SOAR)}\end{aligned}$$

It is clearly that the eigenvalues with the largest magnitude computed by RGAR(10) method is more accurate than SOAR method for this example.

5 Conclusion

We propose in this paper a restarted generalized Arnoldi method and a restarted refined generalized Arnoldi method for solving a large-scale PEP. Approximations to several eigenvalues can be found at the same time. Even though some information is discarded because of restarting, the most

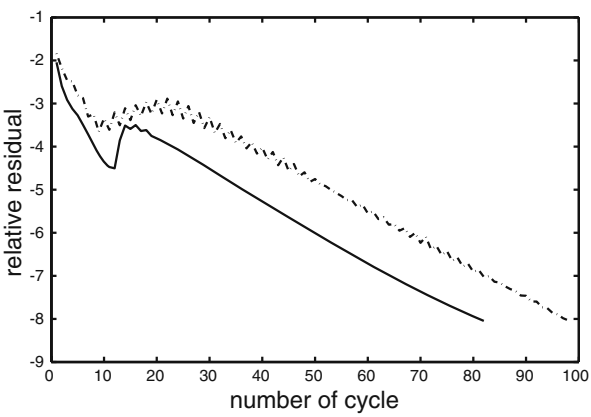

Fig. 3 Convergence plot of GAR(20) (*dash-dot line*) and RGAR(20) (*solid line*)

important information is retained. The methods reduce the large-scale CEP to a small-size CEP by applying the projection technique and also reduce the storage costs by restarting. Numerical tests presented in this paper show the effectiveness of the proposed methods (Fig. 3).

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