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The second-order biorthogonalization procedure and its application to quadratic eigenvalue problems

Bin Wang [a,*], Yangfeng Su [a], Zhaojun Bai [b]

[a] *Department of Mathematics, Fudan University, Shanghai 200433, China*
[b] *Department of Computer Science, University of California, Davis, CA 95616, USA*

Abstract

Given a pair of matrices and starting vectors, we present a procedure to generate the biorthonormal basis of the second-order right and left Krylov subspaces. The application is to solve the large-scale quadratic eigenvalue problems via oblique projection technique. This method can take full advantage of the sparseness of large-scale system as well as the superior convergence behavior of Krylov subspace based methods by implicit linearization, which makes the solution acceptable in terms of both cost and time.

1. Introduction

The Quadratic Eigenvalue Problem (QEP for short) [1] is one of the most important problems that arises in many applications, such as dynamic analysis of structure.

* Corresponding author.
E-mail address: wangb@fudan.edu.cn (B. Wang).

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For simplicity, we write the quadratic λ-matrix of order N as

$$\mathscr{Q}_N(\lambda) = \lambda^2 M + \lambda D + K. \tag{1}$$

M, D, K are given real square matrices of order N. $\lambda \in \mathbb{C}$ is an eigenvalue and nonzero vector x the corresponding right eigenvector of (1) if

$$\mathscr{Q}_N(\lambda)x = (\lambda^2 M + \lambda D + K)x = 0 \tag{2}$$

and nonzero vector y the left eigenvector if

$$y^H \mathscr{Q}_N(\lambda) = y^H(\lambda^2 M + \lambda D + K) = 0. \tag{3}$$

The triplet (λ, x, y) is called the eigentriplet [2] of $\mathscr{Q}_N(\lambda)$.

The common way to solve QEP is first to transform it into an equivalent Generalized Eigenvalue Problem (GEP for short), then any dense methods [3] for GEP should be adopted if all these eigenvalues are desired. For large-scale problems, some iterative methods, for instance, the Jacobi–Davidson method [4,5] which targets at one eigenvalue at a time, and the Krylov subspace based methods [1,6–8] applied to one of its linearization forms, attracted more and more attention in past few years. These approaches suffer some disadvantages, such as solving the GEP of twice order of the original problem and more importantly, the lost of original structures of M, D, K in the process of linearization. Furthermore, essential spectral properties of $\mathscr{Q}_N(\lambda)$ are not guaranteed to preserve.

Recently, a Rayleigh–Ritz projection technique for finding a few eigenvalues, often those with the largest magnitude, and the corresponding eigenvectors of large-scale QEP (2) was proposed in [9]. The remarkable feature in practice is that since this method is applied directly to the original problem, the essential structures of M, D, K as well as the spectral properties are preserved promisingly. The main step is to generate an orthonormal basis of the second-order Krylov subspace by the second-order Arnoldi (SOAR for short) procedure, which can be thought of as a *one-sided* method. In this paper, we extend this idea to the use of a *two-sided* method, which generates two sequences of vectors spanning both the second-order right and left Krylov subspaces. We call it the second-order biorthogonalization (SOB for short) procedure. An oblique projection technique [1,10], which based on a generalized version of the SOB procedure, is applied to QEP and the Ritz triplet (θ, x, y) of $\mathscr{Q}_N(\lambda)$ will be solved at the same time.

Throughout this paper, we use the traditional linear algebra notational convention. By $\|\cdot\|_1$, $\|\cdot\|_2$, and $\|\cdot\|_F$, we denote the 1-, 2- and Frobenius-norm of a vector or matrix. The notation span $\{q_1, q_2, \ldots, q_n\}$, and span $\{Q\}$ stand for the spaces spanned by the vector sequence $\{q_j\}$ and the columns of matrix Q, respectively. Sign of ω is denoted by $\mathrm{sign}(\omega)$.

The rest of this paper is organized as follows. In Section 2, we shall introduce the main procedure to construct the biorthonormal basis of the second-order right and left Krylov subspaces. Then in Section 3, we cover the idea of applying the oblique projection technique to solve the quadratic eigenvalue problems. One numerical example is given in Section 4 to identify our method. We conclude this paper in Section 5.

2. The second-order biorthogonalization procedure

For given A, B and $r_{-1} = 0$, $r_0 = u$, we define the vector sequence $\{r_j\}$ as follows

$$r_j = Ar_{j-1} + Br_{j-2},$$

for $j > 0$. Then, a procedure to generate the orthonormal basis of subspace

$$\mathscr{G}_n(A, B; u) = \mathrm{span}\{r_0, r_1, \ldots, r_{n-1}\},$$

is presented in [9]. We enhance this idea to generate the biorthonormal basis of $\mathscr{G}_n(A, B; u)$ and $\mathscr{G}_n(A^{\mathrm{T}}, B^{\mathrm{T}}; v)$, which we define as *the second-order right and left Krylov subspaces*, i.e., to find the biorthonormal vector sequences $\{q_j\}$ and $\{p_j\}$ such that

$$\begin{aligned} \mathrm{span}\{q_1, q_2, \ldots, q_n\} &= \mathscr{G}_n(A, B; u) \\ \mathrm{span}\{p_1, p_2, \ldots, p_n\} &= \mathscr{G}_n(A^{\mathrm{T}}, B^{\mathrm{T}}; u). \end{aligned} \tag{4}$$

Algorithm 1. The second-order biorthogonalization (SOB) procedure

$\omega = v^{\mathrm{T}} u$
$q_1 = u/\sqrt{|\omega|},\ q_1' = 0$
$p_1 = \mathrm{sign}(\omega) v/\sqrt{|\omega|},\ p_1' = 0$
for $j = 1, 2, \ldots, n$ **do**
  $r = Aq_j + Bq_j',\ r' = q_j$
  $s = A^{\mathrm{T}} p_j + B^{\mathrm{T}} p_j',\ s' = p_j$
  for $i = 1, 2, \ldots, j$ **do**
    $u_{ij} = p_i^{\mathrm{T}} r,\ v_{ij} = s^{\mathrm{T}} q_i$
    $r = r - q_i u_{ij},\ r' = r' - q_i' u_{ij}$
    $s = s - p_i v_{ij},\ s' = s' - p_i' v_{ij}$
  end for
  $\omega = s^T r$
  if $\omega = 0$ **then** *breakdown*
  $u_{j+1,j} = \sqrt{|\omega|},\ v_{j+1,j} = \mathrm{sign}(\omega) u_{j+1,j}$
  $q_{j+1} = r/u_{j+1,j},\ q_{j+1}' = r'/u_{j+1,j}$
  $p_{j+1} = s/v_{j+1,j},\ p_{j+1}' = s'/v_{j+1,j}$
end for

In matrix notation, the above algorithm generates two $N \times n$ matrices Q_n and P_n whose columns are the vector sequences $\{q_j\}$ and $\{p_j\}$, respectively, which satisfy relation (4) and the biorthonormality. The proof is similar to that in [9].

It will be seen above all that the SOB procedure only refer the matrices A and B through the matrix–vector products Ax, $A^{\mathrm{T}}x$ and Bx, $B^{\mathrm{T}}x$. Therefore, A, B do not have to be represented in the usual way as two-dimension arrays of numbers, but as rules to compute the matrix–vector products for any given vector, which is ideal for large-scale and sparse system. This enjoys the same feature as in the standard nonsymmetric Lanczos procedure [11] for generating the biorthonormal basis of $\mathscr{K}_n(A, u)$ and $\mathscr{K}_n(A^{\mathrm{T}}, vu)$. Secondly, the vector sequences $\{q'_j\}$ and $\{p'_j\}$ are auxiliary that must be kept in Algorithm 1, while the memory saving technique in [9] can be adopted to deduce a revision, which removes the requirement of explicit reference of $\{q'_j\}$ and $\{p'_j\}$, as we do in Algorithm 2. Limited by length, we do not explore the details here. Thirdly, if A, B are symmetric matrices, then the above procedure with the same starting vectors yields $Q_n = P_n$ and $U_n = V_n$. It is necessary to compute only one of these two recurrences provided that a symmetric scaling scheme is used at lines 12–16 of Algorithm 1 and the SOB procedure degrades to the SOAR procedure. Fourthly, there are infinitely many ways of choosing the scalars $u_{j+1,j}$ and $v_{j+1,j}$ [12,3] at line 14 of Algorithm 1, as long as they satisfy $\omega = u_{j+i,j}v_{j+i,j}$. There are certain tradeoffs among different choices. Fifthly, this procedure will break down at line 13 when the norm of r or s, or even the inner product of r and s vanishes at a certain step of outer loop. The breakdown of the standard nonsymmetric Lanczos procedure has been discussed extensively; see, for example, [13–15]. But for the second-order case, it is a little difficult to cure such breakdown. This subject is of further study. In this paper, we will always presume that the SOB procedure will not stop prematurely.

3. Oblique projection method for QEP

Before presenting the oblique projection method for QEP, we will first introduce one of the generalized versions of the SOB procedure, which generates the M-biorthonormal basis of subspaces $\mathscr{G}_n(-M^{-1}D, -M^{-1}K; u)$ and $\mathscr{G}_n(-M^{-\mathrm{T}}D^{\mathrm{T}}, -M^{-\mathrm{T}}K^{\mathrm{T}}; v)$.

Algorithm 2. The generalized SOB procedure

1. $\omega = v^{\mathrm{T}}Mu$
2. $q_1 = u/\sqrt{|\omega|},\ p_1 = \mathrm{sign}(\omega)v/\sqrt{|\omega|},$
3. $f = 0$, $g = 0$
4. **for** $j = 1, 2, \ldots, n$ **do**

```
    r = −M^{-1}(Dq_j + Kf), s = −M^{-T}(D^T p_j + K^T g)
    for i = 1, 2, ..., j do
        u_{ij} = p_i^T M r,  r = r − q_i u_{ij}
        v_{ij} = s^T M q_i,  s = s − p_i v_{ij}
    end for
    ω = s^T M r
    if ω = 0 then breakdown
    u_{j+1,j} = sqrt(|ω|), v_{j+1,j} = sign(ω) u_{j+1,j}
    q_{j+1} = r/u_{j+1,j}, p_{j+1} = s/v_{j+1,j},
    f = Q_j Û_j^{-1} e_j,  g = P_j V̂_j^{-1} e_j
end for
```

Matrices $\widehat{U}_j$ and $\widehat{V}_j$ are nonsingular if no breakdown occurs and are defined as

$$\widehat{U}_j = \begin{bmatrix} u_{21} & \cdots & u_{2j} \\ & \ddots & \vdots \\ & & u_{j+1,j} \end{bmatrix} \quad \text{and} \quad \widehat{V}_j = \begin{bmatrix} v_{21} & \cdots & v_{2j} \\ & \ddots & \vdots \\ & & v_{j+1,j} \end{bmatrix}.$$

Given Q_n and P_n, which satisfy $P_n^{\mathrm{T}} M Q_n = I_n$, by Algorithm 2, we can reduce the original quadratic λ-matrix of order N to a small $n \times n$ system by oblique projection technique. Then, the associated QEP is to solve scalar θ and nonzero vectors f and g satisfying

$$\mathcal{Q}_n(\theta) f = (\theta^2 I_n + \theta D_n + K_n) f = 0, \tag{5}$$

$$g^H \mathcal{Q}_n(\theta) = g^H(\theta^2 I_n + \theta D_n + K_n) = 0, \tag{6}$$

where $D_n = P_n^{\mathrm{T}} D Q_n$ and $K_n = P_n^{\mathrm{T}} K Q_n$ are matrices of order n.

The eigentriplet $(\theta, f, g,)$ of $\mathcal{Q}_n(\theta)$ defines the Ritz triplet (θ, x, y), which is the approximating eigentriplet of $\mathcal{Q}_N(\lambda)$, as

$$(\theta, x, y) = (\theta, Q_n f, P_n g). \tag{7}$$

The accuracy can be assessed by the norms of the residual vectors

$$r = (\theta^2 M + \theta D + K)x \quad \text{and} \quad s^H = y^H(\theta^2 M + \theta D + K).$$

The oblique projection method enforces $r \perp \operatorname{span}\{P_n\}$ and $s \perp \operatorname{span}\{Q_n\}$. Moreover, by (7), it is of interest to note that $y^H r = 0$ and $s^H x = 0$. Therefore, we have the following equalities, which measure the backward error for the Ritz triplet (θ, x, y),

$$(\theta^2 M + \theta D + K - E)x = 0 \quad \text{and} \quad y^H(\theta^2 M + \theta D + K - E) = 0, \tag{8}$$

with the backward error matrix $E = rx^H/\|x\|_2^2 + ys^H/\|y\|_2^2$. If norm of E, i.e.,

$$\|E\|_F^2 = \frac{\|r\|_2^2}{\|x\|_2^2} + \frac{\|s\|_2^2}{\|y\|_2^2}, \tag{9}$$

is small enough, then by (8) we conclude that the Ritz triplet, (θ, x, y) is the exact eigentriplet of a slightly perturbed λ-matrix of $\mathcal{Q}_N(\lambda)$ [16].

A high level description of the oblique projection method based on the generalized SOB procedure for solving QEP are given as follows.

Algorithm 3. Oblique projection method for QEP

1. Run the generalized SOB procedure with matrices M, D, K and starting vectors u, v to construct the $N \times n$ M-biorthonormal matrices Q_n and P_n.
2. Reduce the system by computing $D_n = P_n^{\mathrm{T}} D Q_n$ and $K_n = P_n^{\mathrm{T}} K Q_n$.
3. Solve the reduced QEP (5) and (6) for eigentriplet (θ, f, g) and obtain the Ritz triplet (θ, x, y) with $x = Q_n f/\|Q_n f\|_2$ and $y = P_n g/\|P_n g\|_2$.
4. Assess the accuracy of the Ritz triplet by the relative norms of residual vectors as

$$\frac{\|(\theta^2 M + \theta D + K)x\|_2}{|\theta|^2\|M\|_1 + |\theta|\|D\|_1 + \|K\|_1} \quad \text{and} \quad \frac{\|y^H(\theta^2 M + \theta D + K)\|_2}{|\theta|^2\|M\|_1 + |\theta|\|D\|_1 + \|K\|_1}. \tag{10}$$

Since in line 5 of the generalized SOB procedure, we would solve $Mx = b$ or $M^{\mathrm{T}}x = b$ for any right hand side b, it is ideal to provide a factorization form of M, for example LU factorization before entering the outer loop of Algorithm 2 for computational efficiency. Secondly, we should note that if M, D, K are symmetric matrices, then the generalized SOB procedure with the same starting vectors yields $Q_n = P_n$. Therefore, the reduced matrices D_n and K_n are also symmetric, too. Thus, the essential structures of the original system are explicitly preserved and the spectral properties may also be preserved in the reduced one. Thirdly, for solving the reduced QEP in step 3 of Algorithm 3, we use the dense approach mentioned in Section 1. In practice, the reduced order n is considerably smaller than the order N of the original problem, hence a substantial computational effort can be eliminated by solving the reduced QEP instead of the original one.

4. Numerical experiment

In this section, we give a numerical experiment to verify that our oblique projection method Algorithm 3 (*GSOB*) can solve QEP promisingly. The results reported are compared with the exact eigenvalues (*Exact*) computed by

MATLAB function **polyeig**, and the approximating eigenpairs by the SOAR method (*SOAR*). In this example, M, D, K are 200×200 random nonsymmetric matrices. The starting vectors are chosen to be vectors with all components equal to 1 and the breakdown threshold to be 10^{-10}.

The left plot of Fig. 1 shows the approximate eigenvalues computed with reduced order $n = 20$. The right plot of Fig. 1 shows the relative norms of the right (*GSOB right*) and left (*GSOB left*) residual vectors computed by Eq. (10) as well as the norms of the backward error matrices (*Error Matrix*) by (9). We can conclude that the convergence behaviors of both the right and left Ritz vectors are essentially the same, and the Ritz triplets are the exact eigentriplets of $\mathcal{Q}_N(\lambda)$ plus error matrices in small norm.

To show that Ritz values converge to the exact eigenvalues, often those with the largest magnitude, we plot the relative error of the eigenvalue with the largest magnitude ($\lambda = -32.2 \pm 15.5i$) in the left plot of Fig. 2, and that of the

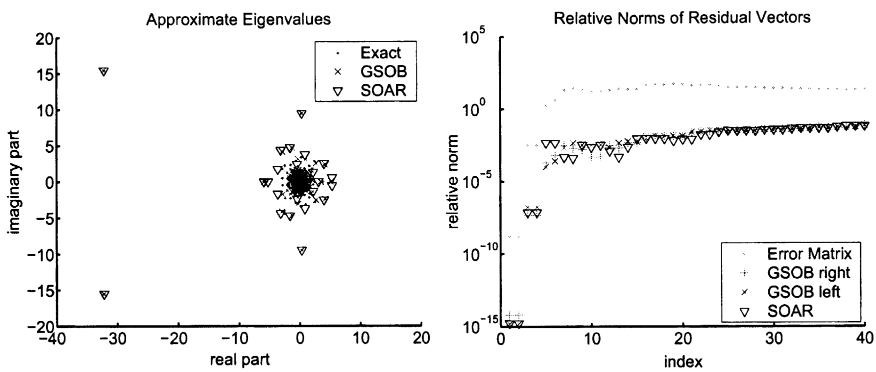

Fig. 1. Approximate eigenvalues and relative norms.

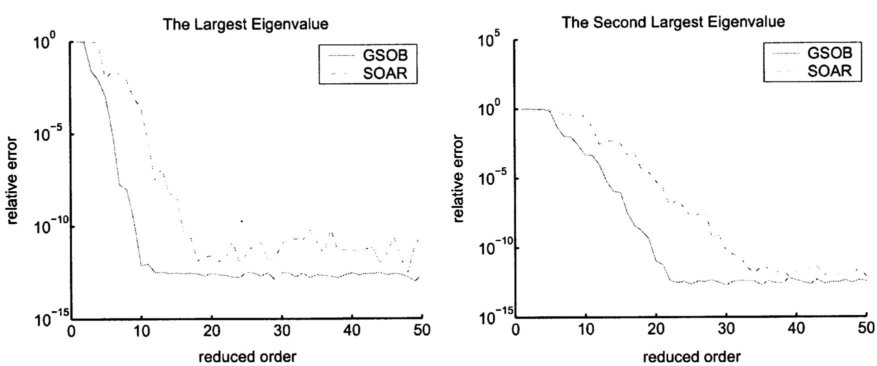

Fig. 2. Relative error of eigenvalues.

second largest eigenvalue ($\lambda = 0.307 \pm 9.43i$) in the right plot of Fig. 2 with respect to the reduced order n from 1 to 50. The convergence behavior of SOAR are also plotted in Fig. 2. It is easy to see that GSOB converges to the exact eigenvalues faster than SOAR for this example.

Other numerical experiments, not presented here, also verify that some Ritz values and the corresponding Ritz vectors of the reduced QEP are very good approximations to the exact ones with the largest magnitude of the original problem.

5. Conclusion

This article introduces a SOB procedure, which generates the biorthonormal basis of the second-order right and left Krylov subspaces. A generalized version of this procedure is applied to solve QEP via oblique projection technique. Therefore, the original large-scale system is reduced to a small one, which can be solved with dense methods. In practice, the order of the reduced problem is considerably smaller than that of the original problem, hence a substantial computational efforts can be eliminated by solving the reduced QEP instead of the original one. Because of implicit linearization, the superior convergence behavior of Krylov subspace based methods is also achieved.

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