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A NOVEL DEFLATION TECHNIQUE FOR SOLVING QUADRATIC EIGENVALUE PROBLEMS

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Abstract

In this paper we propose numerical algorithms for solving large-scale quadratic eigenvalue problems for which a set of eigenvalues closest to a fixed target and the associated eigenvectors are of interest. The desired eigenvalues are usually with smallest modulo in the spectrum. The algorithm based on the quadratic Jacobi-Davidson (QJD) algorithm is proposed to find the first smallest eigenvalue closest to the target. To find the successive eigenvalues closest to the target, we propose a novel explicit non-equivalence low-rank deflation technique. The technique transforms the smallest eigenvalue to infinity, while all other eigenvalues remain unchanged. Thus, the original second smallest eigenvalue becomes the smallest of the new quadratic eigenvalue problem, which can then be solved by the QJD algorithm. To compare with locking and restarting quadratic eigensolver, our numerical experience shows that the QJD method combined with our explicit non-equivalence deflation is robust and efficient.

1. Introduction

Deflation technique is an important concept for solving eigenvalue problems. Suppose that we have computed some eigenvalues and their associated eigenvectors or Schur vectors of an input matrix or pair by some iterative algorithms. Those algorithms always deliver a few eigenvalues which are closest to a certain target along with their eigen- or Schur vectors. The problem now becomes to how to compute the next few eigenpairs which are

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closest to the certain target by the same algorithms. To restart with a differently selected Ritz pair, in general, with no guarantee that this algorithm leads to a new eigenpairs close to the target. A well-known way out of this problem is to use a technique, known as deflation.

For solving linear eigenvalue problems, an old technique-Wielandt deflation [16, Chap. 4 & 9], typically a low-rank modification, is applied to the original matrix pair so as to displace the computed eigenvalues, while keeping all other eigenvalues unchanged. The low rank modification is chosen so that the uncomputed desired eigenvalue becomes the one with closest modulus to the target of the modified matrix pair, and therefore, the proposed algorithm can now be applied to the new matrix pair to extract the new desired eigenpairs. This low rank modified matrix pair by Wielandt deflation is typically not equivalent to the original matrix pair.

Recently, some elaborate deflation techniques based on the existence of a Schur decomposition of a matrix pair are proposed for solving eigenvalue problems. Those deflation techniques such as locking and purging are developed to incorporate with implicitly restarted, shift-and-invert, Arnoldi- or Lanczos-type algorithms [10, 11, 12, 13, 24, 25], as well as Jacobi-Davidson-type algorithms [21, 22] for solving standard and generalized eigenvalue problems.

In this paper, we are interested in solving a few eigenpairs (λ, x) close to a certain target of the Quadratic Eigenvalue Problem (QEP)

$$Q(\lambda)x := (\lambda^2 M + \lambda C + K)x = 0, \tag{1.1}$$

where M, C and K are $n \times n$ symmetric real matrices with M and K being positive definite. Typically, M and K represent the mass and stiffness matrices, respectively, and C represents the damping matrix of the system. QEPs of (1.1) arise in the solution of initial or boundary value problems for second order systems of the form

$$M\ddot{q} + C\dot{q} + Kq = f \tag{1.2}$$

and in other applications. These include finite element characterization in structural analysis [18], and in acoustic simulation of poro-elastic materials [15, 17, 19]. See also [28] for a recent survey. The classical approach in

solving the QEP is to transform it into a generalized eigenvalue problem by introducing a new vector $y = \lambda x$:

$$\left(\begin{bmatrix} 0 & I \\ K & C \end{bmatrix} - \lambda \begin{bmatrix} I & 0 \\ 0 & -M \end{bmatrix} \right) \begin{bmatrix} x \\ y \end{bmatrix} = 0. \tag{1.3}$$

If $(\lambda, \begin{bmatrix} x \\ y \end{bmatrix})$ is an eigenpair of (1.3), then x is an eigenvector of (1.1) corresponding to the eigenvalue λ. The approach in (1.3) allow us to determine eigenpairs numerically, since for the generalized eigenvalue problem (1.3) the mathematical theory, numerical methods as well as the perturbation theory are well established [1, 5, 26]. However, due to the embedding into the problem of double size, and the destroying of the specific zero, identity blocks and the symmetric structure of (1.3) by perturbation, the condition numbers of the eigenvalues and eigenvectors with respect to perturbations in the data M, C, K may increase [27, 28]. In view of this remark it would be ideal to develop a numerical algorithm that works directly with the original data of the quadratic eigenvalue problem for avoiding the problem of the increased condition numbers.

A comment on quadratic or general higher-order eigenvalue problem by Bai [2] says "besides transforming such an eigenvalue problem to the standard eigenvalue problem, not much progress has been made concerning how to solve such λ-matrix eigenvalue problem directly and efficiently". The recent proposed quadratic or polynomial Jacobi-Davidson methods [7, 20, 23] partially fulfill these requirements. The methods use projections on low-dimensional subspaces in order to reduce the given polynomial eigenproblem to a polynomial eigenproblem with matrix coefficients of lower order. The reduced problem can then be solved by standard methods.

The quadratic or polynomial Jacobi-Davidson methods [20, 23] proposed a shift-target strategy for possibly computing interior eigenvalues without inversion. However, if the desired eigenvalues of (1.1) form a cluster of nearby eigenvalues, then the quadratic Jacobi-Davidson method sometimes has difficulties in detecting and resolving such a cluster. The undesired effect is that in this case for different starting eigenpairs it converges to the same eigenpair of (1.1). It is know that implicit deflation technique based on Schur forms (See e.g. §4.7 and §8.4 of [3]) combined with Jacobi-Davidson method

performs well for the linear eigenvalue problem. However, in the quadratic or high-order eigenvalue problem, it is not clear how to incorporate an implicit deflation technique because a Schur form , in general, does not exist to a quadratic or a polynomial pencil.

A very recently proposed locking and restarting quadratic eigensolver [14] gives the link between methods for solving quadratic eigenproblems and the linearized problem. It combines the benefits of the quadratic and the linearized approaches by employing a locking and restarting scheme based on the partial Schur form of the linearized problem in quadratic Jacobi-Davidson method. This method essentially locks the desired eigenvalues in a reduced quadratic pencil by an equivalence projection. In this case, some dummy (meaningless) Ritz values will appear in the reduced quadratic eigenproblem and possibly disturb the selection of the new desired eigenvalues.

In this paper, we will develop an explicit non-equivalence low-rank deflation technique based on the method proposed in [6, 9] for quadratic eigenproblem. Suppose that (λ_1, x_1) is a given eigenpair. The new deflation technique transforms the original quadratic eigenproblem (1.1) to a new deflated quadratic eigenproblem so that it has an infinite eigenvalue transformed from λ_1 and keep the remaining eigenpairs invariant.

2. Non-Equivalence Low-Rank Deflation

In this section, we will construct a new non-equivalence low-rank deflated quadratic pencil $\tilde{Q}(\lambda) := \lambda^2\tilde{M} + \lambda\tilde{C} + \tilde{K}$ such that a given isolated eigenmatrix pair $(\Lambda_1, X_1) \in \mathbb{R}^{r\times r} \times \mathbb{R}^{n\times r}$ of the quadratic pencil $Q(\lambda) := \lambda^2 M + \lambda C + K$ is replaced by $(\mathrm{diag}_r\{\infty, \ldots, \infty\}, X_1)$, while the other eigenvalues and the associated eigenvectors are kept invariant. Here the subindex r in diag_r denotes the dimension of the diagonal matrix.

Definition 2.1. Let $Q(\lambda) := \lambda^2 M + \lambda C + K$ be a quadratic pencil as in (1.1), and $(\Lambda_1, X_1) \in \mathbb{R}^{k\times k} \times \mathbb{R}^{n\times k}$ be a given pair, where X_1 is of full column rank. The pair (Λ_1, X_1) is called an eigenmatrix pair of $Q(\lambda)$ if it satisfies

$$MX_1\Lambda_1^2 + CX_1\Lambda_1 + KX_1 = 0. \tag{2.1}$$

In particular, $(\mathrm{diag}_k\{\infty, \ldots, \infty\}, X_1)$ is called an "infinity" eigenmatrix pair of $Q(\lambda)$ if $MX_1 = 0$.

Note that if $k = 1$ then $\lambda_1 = \Lambda_1$ is called an eigenvalue of $Q(\lambda)$ and $x_1 = X_1$ is the associated eigenvector. And (λ_1, x_1) is called an eigenpair of $Q(\lambda)$.

Theorem 2.1. *Given an eigenmatrix pair* $(\Lambda_1, X_1) \in \mathbb{R}^{r\times r} \times \mathbb{R}^{n\times r}(r \le n)$ *of* $Q(\lambda) := \lambda^2 M + \lambda C + K$, *where* Λ_1 *is nonsingular and* X_1 *satisfies*

$$X_1^T K X_1 = I_r, \qquad \Theta_1 := (X_1^T M X_1)^{-1}. \tag{2.2}$$

We define

$$\tilde{M} := M - M X_1 \Theta_1 X_1^T M, \tag{2.3}$$

$$\tilde{C} := C + M X_1 \Theta_1 \Lambda_1^{-T} X_1^T K + K X_1 \Lambda_1^{-1} \Theta_1 X_1^T M, \tag{2.4}$$

$$\tilde{K} := K - K X_1 \Lambda_1^{-1} \Theta_1 \Lambda_1^{-T} X_1^T K. \tag{2.5}$$

Suppose that $\Theta_1 - \Lambda_1 \Lambda_1^T$ *is nonsingular. Then the real symmetric pencil* $\tilde{Q}(\lambda) := \lambda^2 \tilde{M} + \lambda \tilde{C} + \tilde{K}$ *has the following spectral property: the eigenvalues of the quadratic pencil* $\tilde{Q}(\lambda)$ *are the same as those of* $Q(\lambda)$ *except that the eigenvalues of* Λ_1, *which are closed under complex conjugation, are replaced by* r *infinities.*

Proof. By assumption and definition 2.1 we see that (Λ_1, X_1) is an eigenmatrix pair of $Q(\lambda)$ and satisfies

$$M X_1 \Lambda_1^2 + C X_1 \Lambda_1 + K X_1 = 0. \tag{2.6}$$

Then from (2.6) we have

$$\begin{aligned} \tilde{Q}(\lambda) &:= \lambda^2 \tilde{M} + \lambda \tilde{C} + \tilde{K} + \lambda (M X_1 \Theta_1 \Lambda_1^{-T} X_1^T K + K X_1 \Lambda_1^{-T} \Theta_1^{-1} \Theta_1 X_1^T M) \\ &\quad - K X_1 \Lambda_1^{-1} \Theta_1 \Lambda_1^{-T} X_1^T K \\ &= Q(\lambda) + (M X_1 (\lambda I_r + \Lambda_1) + C X_1) \Theta_1 \Lambda_1^{-T} (X_1^T K - \lambda \Lambda_1^T X_1^T M) \\ &= Q(\lambda) + Q(\lambda) X_1 (\lambda I_r - \Lambda_1)^{-1} \Theta_1 \Lambda_1^{-T} (X_1^T K - \lambda \Lambda_1^T X_1^T M). \end{aligned} \tag{2.7}$$

By using the identity

$$\det(I_n + RS) = \det(I_m + SR),$$

where $R, S^T \in \mathbb{R}^{n\times m}$, and (2.7) we have

$$\begin{aligned}\det[\tilde{Q}(\lambda)] &= \det[Q(\lambda) + Q(\lambda)X_1(\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(X_1^TK - \lambda\Lambda_1^TX_1^TM)]\\ &= \det[Q(\lambda)]\det[I_r + (\lambda I_r - \Lambda_1)^{-1}\Theta_1\Lambda_1^{-T}(I_r - \lambda\Lambda_1^T\Theta_1^{-1})]\\ &= \frac{\det[Q(\lambda)]}{\det(\lambda I_r - \Lambda_1)}\det(\Theta_1\Lambda_1^{-T} - \Lambda_1). \qquad (2.8)\end{aligned}$$

Since $(\Theta_1 - \Lambda_1\Lambda_1^T) \in \mathbb{R}^{r\times r}$ is nonsingular, we have $\det(\Theta_1\Lambda_1^{-T} - \Lambda_1) \neq 0$. Therefore, $\tilde{Q}(\lambda)$ has the same eigenvalues as $Q(\lambda)$ except that r eigenvalues of Λ_1 are replaced by r infinities. □

In accordance of Theorem 2.1 we can deflate r unwanted eigenvalues of Λ_1, which are closed under complex conjugation, by using real arithmetic. That means we can obtain the new non-equivalence low-rank deflated quadratic pencil $\tilde{Q}(\lambda)$, without adopting any complex arithmetic, when unwanted eigenvalues of Λ_1 are replaced by r infinities.

Next, we show that the remaining eigenpairs of $Q(\lambda)$ keep invariant on deflating. Based on the observation of [4] we prove the following orthogonality relation.

Lemma 2.1. *Let* $(\Lambda_1, X_1) \in \mathbb{R}^{r\times r}\times\mathbb{R}^{n\times r}$ *and* $(\Lambda_2, X_2) \in \mathbb{R}^{s\times s}\times\mathbb{R}^{n\times s}$ *be two eigenmatrix pairs of* $Q(\lambda)$ *with* $X_1^TKX_1 = I_r$ *and* $X_2^TKX_2 = I_s$. *Suppose that* $\mathrm{spec}(\Lambda_1) \cap \mathrm{spec}(\Lambda_2) = \emptyset$. *Then the orthogonality relation holds*

$$X_2^TKX_1 = \Lambda_2^T(X_2^TMX_1)\Lambda_1. \qquad (2.9)$$

Proof. Assumption gives the equations

$$X_2^TMX_1\Lambda_1^2 + X_2^TCX_1\Lambda_1 + X_2^TKX_1 = 0, \qquad (2.10)$$

$$(\Lambda_1^T)^2X_2^TMX_1 + \Lambda_2^TX_2^TCX_1 + X_2^TKX_1 = 0. \qquad (2.11)$$

Eliminating term involving "$X_2^TCX_1$" by multiplying (2.10) and (2.11) by Λ_2^T from the left and by Λ_1 from the right, respectively, we obtain

$$\Lambda_2^T(X_2^TMX_1)\Lambda_1^2 - (\Lambda_2^T)^2(X_2^TMX_1)\Lambda_1 + \Lambda_2^T(X_2^TKX_1) - (X_2^2KX_1)\Lambda_1 = 0. \qquad (2.12)$$

Let $M_X := X_2^T M X_1, K_X := X_2^T K X_1$. Then vectorizing the equation (2.12) we have

$$\begin{aligned}(I_r \otimes \Lambda_2^T - \Lambda_1^T \otimes I_s)\mathrm{vec}(K_X) &= \mathrm{vec}(\Lambda_2^T(\Lambda_2^T M_X - M_X\Lambda_1)\Lambda_1)\\ &= (\Lambda_1^T \otimes \Lambda_2^T)\mathrm{vec}(\Lambda_2^T M_X - M_X\Lambda_1)\\ &= (\Lambda_1^T \otimes \Lambda_2^T)(I_r \otimes \Lambda_2^T - \Lambda_1^T \otimes I_s)\mathrm{vec}(M_X)\\ &= (I_r \otimes \Lambda_2^T - \Lambda_1^T \otimes I_s)(\Lambda_1^T \otimes \Lambda_2^T)\mathrm{vec}(M_X). \quad (2.13)\end{aligned}$$

Here $\otimes$ denotes the Kronecker product of two matrices. Since $\mathrm{spec}(\Lambda_1) \cap \mathrm{spec}(\Lambda_2) = \emptyset$, the matrix $(I_r \otimes \Lambda_2^T - \Lambda_1^T \otimes I_s)$ is nonsingular, and hence $(\Lambda_1^T \otimes \Lambda_2^T)(\mathrm{vec}(M_X)) = \mathrm{vec}(K_X)$ by (2.13). Thus, the orthogonality relation (2.9) holds. □

Theorem 2.2. *Let $(\Lambda_2, X_2) \in \mathbb{R}^{s\times s} \times \mathbb{R}^{n\times s}$ be an eigenmatrix pair of $Q(\lambda)$ with $X_2^T K X_2 = I_s$ and $\tilde{Q}(\lambda) := \lambda^2\tilde{M} + \lambda\tilde{C} + \tilde{K}$ be given in Theorem 2.1. Suppose $\mathrm{spec}(\Lambda_1) \cap \mathrm{spec}(\Lambda_2) = \emptyset$. Then (Λ_2, X_2) is also an eigenmatrix pair of $\tilde{Q}(\lambda)$.*

Proof. Since (Λ_2, X_2) is an eigenmatrix pair of $Q(\lambda)$, we have

$$MX_2\Lambda_2^2 + CX_2\Lambda_2 + KX_2 = 0. \quad (2.14)$$

From (2.3)−(2.5) follows that

$$\begin{aligned}&\tilde{M}X_2\Lambda_2^2 + \tilde{C}X_2\Lambda_2 + \tilde{K}X_2\\ &= (M - MX_1\Theta_1X_1^TM)X_2\Lambda_2^2 + (C + MX_1\Theta_1\Lambda_1^{-T}X_1^TK\\ &\quad + KX_1\Lambda_1^{-1}\Theta_1X_1^TM)X_2\Lambda_2 + (K - KX_1\Lambda_1^{-1}\Theta_1\Lambda_1^{-T}X - 1^TK)X_2\\ &= MX_2\Lambda_2^2 - MX_1\Theta_1X_1^TMX_2\Lambda_2^2 + CX_2\Lambda_2 + MX_1\Theta_1\Lambda_1^{-T}X_1^TKX_2\Lambda_2\\ &\quad + KX_1\lambda_1^{-1}\Theta_1X_1^TMX_2\Lambda_2 + KX_2 - KX_2\Lambda_1^{-1}\Theta_1\Lambda_1^{-T}X_1^TKX_2\\ &= -MX_1\Theta_1X_1^TMX_2\Lambda_2^2 + MX_1\Theta_1\Lambda_1^{-T}X_1^TKX_2\Lambda_2\\ &\quad + KX_1\lambda_1^{-1}\Theta_1X_1^TMX_2\Lambda_2 - KX_2\Lambda_1^{-1}\Theta_1\Lambda_1^{-T}X_1^TKX_2\\ &= MX_1\Theta_1\Lambda_1^{-T}(X_1^TKX_2\Lambda_2 - \Lambda_1^TX_1^TMX_2\Lambda_2^2)\\ &\quad + KX_1\Lambda_1^{-1}\Theta_1\Lambda_1^{-T}(\Lambda_1^TX_1^TMX_2\Lambda_2 - X_1^TKX_2). \quad (2.15)\end{aligned}$$

From the orthogonality relation in Lemma 2.1 the assertion follows. □

Remark 2.1. (a) Let $(\lambda_1 := \alpha_1 + i\beta_1, x_1)$ be an isolated complex eigenpair of $Q(\lambda)$ i.e., $Q(\lambda_1)x_1 = 0$, with $\alpha_1, \beta_1 \neq 0 \in \mathbb{R}$ and $x_1 = x_{1R} + ix_{1I}, x_{1R}, x_{1I} \in \mathbb{R}^n$. Since $(\overline{\lambda}_1, \overline{x}_1)$ is also an eigenpair of $Q(\lambda)$, we have

$$M\underline{X}_1\underline{\Lambda}_1^2 + C\underline{X}_1\underline{\Lambda}_1 + K\underline{X}_1 = 0, \tag{2.16}$$

where

$$\underline{\Lambda}_1 = \begin{bmatrix} \alpha_1 & \beta_1 \\ -\beta_1 & \alpha_1 \end{bmatrix} \quad \text{and} \quad \underline{X}_1 = \begin{bmatrix} x_{1R} & x_{1I} \end{bmatrix} \tag{2.17}$$

Suppose that $\underline{X}_1 = [x_{1R}, x_{1I}]$ is of full column rank. Since K is positive definite, there is an orthogonal matrix $S_1 \in \mathbb{R}^{2\times 2}$ such that

$$S_1^T(\underline{X}_1^T K \underline{X}_1)S_1 = D_1^2 = \begin{bmatrix} d_1^2 & 0 \\ 0 & d_2^2 \end{bmatrix} > 0. \tag{2.18}$$

Let

$$\Lambda_1 = D_1 S_1^T \underline{\Lambda}_1 S_1 D_1^{-1} = \begin{bmatrix} \alpha_1 & \frac{\beta_1 d_1}{d_2} \\ -\frac{d_2\beta_1}{d_1} & \alpha_1 \end{bmatrix} \tag{2.19}$$

and

$$X_1 = \underline{X}_1 S_1 D_1^1. \tag{2.20}$$

Then $(\lambda_1, X_1) \in \mathbb{R}^{2\times 2} \times \mathbb{R}^{n\times 2}$ is a complex conjugate eigenpair of $Q(\lambda)$ with $X_1^T K_1 X_1 = I_2$. The non-equivalence low-rank deflation formulae (2.3)−(2.5) now can be applied to the eigenpair (Λ_1, X_1).

(b) The degenerate case, where the real and imaginary parts of eigenvectors, x_{1R} and x_{1I} are linearly dependent, can occur for quadratic pencil $Q(\lambda)$. In this case, the eigenvector x_1 corresponding to $\lambda_1 \in \mathbb{C}$ can be a real vector scaling by a complex number $\frac{\ell - i}{2\ell\|x_{1R}\|_2}$ provided $x_{1I} = \ell x_{1R}$. Since both (λ_1, x_1) and $(\overline{\lambda}_1, x_1)$ are eigenpairs of $Q(\lambda)$, we have

$$\lambda_1^2 M x_1 + \lambda_1 C x_1 + K x_1 = 0, \tag{2.21}$$

$$\overline{\lambda}_1^2 M x_1 + \overline{\lambda}_1 C x_1 + K x_1 = 0. \tag{2.22}$$

Then we obtain $(\lambda_1 + \overline{\lambda}_1)Mx_1 + Cx_1 = 0$. This implies that Cx_1 is parallel to Mx_1, and thus, Kx_1 is parallel to Mx_1. Let $Q \in \mathbb{R}^{n\times n}$ be an orthogonal

matrix such that $Q^T x_1 = e_1$. When we let

$$\tilde{M} = Q^T M Q, \qquad \tilde{C} = Q^T C Q, \qquad \tilde{K} = Q^T K Q,$$

we can see that the first columns and rows of $\tilde{M}, \tilde{C}$ and $\tilde{K}$ are mutually parallel. Hence if we apply Gaussian elimination, say L and L^T, to eliminate those elements from the second component to the nth component of the first column and the first row of $\tilde{M}$, respectively, the dimension of the quadratic eigenproblem can be reduced to $n-1$, whenever we deflate the first column and row of matrices $L\tilde{M}L^T, L\tilde{C}L^T$ and $L\tilde{K}L^T$ simultaneously.

3. Quadratic Jacobi-Davidson Algorithm and Deflation

As mentioned in Section 1 the possible disadvantage of the linearized approach for the QEP in (1.1) are the doubling of the dimension of the problem and the increasing of the condition numbers of eigenpairs. The quadratic Jacobi-Davidson method [20, 23] proposed a shift-target strategy for possibly computing interior eigenvalues without inversion. In this method, the QEP is first projected onto a low-dimensional subspace, which leads to a QEP of modest dimension. This low-dimensional projected QEP can be solved with any method of choice. Expansion of the subspace is realized by a Jacobi-Davidson correction equation.

In the first part of the quadratic Jacobi-Davidson iteration step for solving the QEP of (1.1), the projected quadratic eigenproblem onto the search subspace span(V)

$$(\rho^2 V^T M V + \rho V^T C V + V^T K V)y = 0. \tag{3.1}$$

The columns of $n \times m$ real matrix V are constructed to be orthogonal for stability reasons. The projected problem (3.1) is typically of much smaller dimension with $m \ll n$. First, a Ritz value ρ with desired properties, such as the largest real part or closest to a given target τ_0, is selected and for the associated eigenvector y with $\| y \|_2 = 1$. Then the Ritz vector $u \equiv Vy$ and the residual $r = Q(\rho)u$ is computed. For expansion of the search space the vector p,

$$p := Q'(\rho)u = (2\rho C + K)u \tag{3.2}$$

is also computed.

In the second part of the quadratic Jacobi-Davidson iteration step, the search subspace span(V) is expanded by a vector $\hat{t} \perp u$ that solves (approximately) the correction equation

$$\left(I - \frac{pu^H}{u^H p}\right) Q(\rho)(I - uu^H)t = -r. \tag{3.3}$$

In order to maintain the computation of the projected eigenproblem in (3.1) in real arithmetic, the next columns of the new V are obtained by orthonormalizing the approximate solutions $\mathrm{Re}(\hat{t})$ and $\mathrm{Im}(\hat{t})$ sequentially against the previously computed columns of V whenever the approximate solution t is a complex vector, otherwise by orthonormalizing the approximate solution $\hat{t}$ against the columns of V. This approach is repeated until a desired eigenpair (λ_1, x_1) has been computed, i.e., until the residual r is sufficiently small.

Once a desired eigenpair (λ_1, x_1) has been detected, we can use the non-equivalence low-rank deflation given by Section 2 to transform the computed eigenvalue to infinity so that the next desired eigenvalue becomes the closest eigenvalue to the target. Thus, the above quadratic Jacobi-Davidson process can be repeatedly used for computing the new desired eigenpairs.

We now consider two cases of real eigenvalues or complex conjugate eigenvalues. Suppose that we have computed a real eigenvalue λ_1 and the associated real eigenvector x_1 with $x_1^T K x_1 = 1$ satisfying $Q(\lambda_1)x_1 = 0$. Let $\theta_1 = (x_1^T M x_1)^{-1}$. As in (2.3)−(2.5) we define a new deflated quadratic eigenproblem $\tilde{Q} := \lambda^2\tilde{M} + \lambda\tilde{C} + \tilde{K}$ by

$$\tilde{M} = M - \theta_1 M x_1 x_1^T M \tag{3.4}$$

$$\tilde{C} = C + \frac{\theta_1}{\lambda_1}(M x_1 x_1^T K + K x_1 x_1^T M) \tag{3.5}$$

$$\tilde{K} = K - \frac{\theta_1}{\lambda_1^2} K x_1 x_1^T K. \tag{3.6}$$

Suppose that we have computed a complex eigenvalue $\lambda_1 = \alpha_1 + i\beta_1$, and the associated eigenvector $x_1 = x_{1R} + ix_{1I}$ such that $Q(\lambda_1)x_1 = 0$. Let $\Theta_1 = (X_1^T M X_1)^{-1}$, where $X_1 = [x_{1R}, x_{1I}]$. Then from (2.16)−(2.20) we define a new deflated quadratic eigenproblem $\tilde{Q}(\lambda) = \lambda^2\tilde{M} + \lambda\tilde{C} + \tilde{K}$ by

$$\tilde{M} = M - M X_1 \Theta_1 X_1^T M \tag{3.7}$$

$$\tilde{C} = C + MX_1\Theta_1\Lambda_1^{-T}X_1^TK + KX_1\Lambda_1^{-1}\Theta_1^TX_1^TM) \quad (3.8)$$

$$\tilde{K} = K - KX_1\Lambda_1^{-1}\Theta_1\Lambda_1^{-T}X_1^TK. \quad (3.9)$$

in which $\Lambda_1 = \begin{bmatrix} \alpha_1 & \beta_1 \\ -\beta_1 & \alpha_1 \end{bmatrix}$.

Using this deflation technique we now present the ingredients for our algorithm. We solve the QEP in (1.1) by the quadratic Jacobi-Davidson method [3, 23] combined with the non-equivalence low-rank deflation technique (3.4) or (3.7). We summarize this approach in the following algorithm.

Algorithm 3.1. (*Quadratic Jacobi-Davidson Algorithm + Non-equivalence Low-rank Deflation*)

Input: *Matrices $C_2 = M, C_1 = C, C_0 = K$ as in (1.1). A target τ_0 with nonnegative imaginary part and a number ℓ of desired eigenpairs nearest to τ_0. Positive integer numbers $\ell + 2 \le m_{min} \le m_{max}$ for the minimal and maximal dimensions of the search subspaces. Tolerance "Tol" for the stopping criterion. Choose randomly a $n \times m_{min}$ real matrix $V \in \mathbb{R}^{n\times m_{min}}$.*

Output: *The ℓ desired eigenpairs $\{(\lambda_j, x_j)\}_{j=1}^{\ell}$ of*

$$Q(\lambda)x = (\lambda^2M + \lambda C + K)x = 0,$$

associated with eigenvalues $\{\lambda_j\}_{j=1}^{\ell}$ that are nearest to the target τ_0.

While $(j \le \ell)$ *do*

I. Start: let $m = m_{min}$ and $j = 1$. Orthonormalize V.

II. Repeat:

(i) Compute $H_2 \leftarrow V^TMV, \quad H_1 \leftarrow V^TCV, \quad H_0 \leftarrow V^TKV$.

(ii) Compute m_{min} eigenpairs $\{(\rho_i, y_i)\}_{i=1}^{m_{min}}$ of

$$(\rho^2H_2 + \rho H_1 + H_0)y = 0,$$

where $\|y_i\|_2 = 1$ and ρ_i has nonnegative imaginary part so that the eigenvalues $\{\rho_i\}_{i=1}^{m_{min}}$ are nearest to the target τ_0 satisfying

$$|\rho_{m_{min}} - \tau_0| \ge \cdots \ge |\rho_1 - \tau_0|.$$

(iii) Compute $u \leftarrow Vy_1, \quad p \leftarrow (2\rho_1 C_2 + C_1)u, \quad \{v_i \leftarrow Vy_i\}_{i=2}^{m_{min}}$.

(iv) Compute $r \leftarrow (\rho_1^2 M + \rho_1 C + K)u$.

(v) If $(\|r\|_2 < Tol)$, *then*

$\lambda_j = \rho_1 \ (Im(\rho_1) \geq 0), \ x_j = u$

If λ_j *is real, then* $j = j + 1$; *else* $j = j + 2$.

Else

(v.1) Solve (approximately) a $\hat{t} \perp u$ *from*

$$(I - \frac{pu^H}{u^H p})Q(\rho_1)(I - uu^H)t = -Q(\rho_1)u \equiv -\tilde{r}. \qquad (3.10)$$

(v.2) Expand V:

$V \leftarrow ModGS([V|\hat{t}]), \ m = m + 1, \ if \ \hat{t} \in \mathbb{R}^n$;

$V \leftarrow ModGS([V|Re(\hat{t}), Im(\hat{t})]), \ m = m + 2, \ if \ \hat{t} \in \mathbb{C}^n$.

(v.3) (Restart)

If $m > M_{max}$, *then*

Set $i = 2$.

If $u \in \mathbb{R}^n$, *then* $V = [u], \ m = 1$; *else* $V = [Re(u), Im(u)], \ m = 2$.

While $(m \leq m_{min})$ *do*

$V \leftarrow ModGS([V|v_i]), \ m = m + 1, \ i = i + 1, \ if \ v_i \in \mathbb{R}^n$;

$V \leftarrow ModGS([V|Re(v_i), Im(v_i)]), \ m = m + 2, \ i = i + 1, \ if \ v_i \in \mathbb{C}^n$.

end while m

End if

Go to Repeat

End if.

(vi) (Deflation) Select a new suitable target τ_0.

If λ_j *is real, then compute*

$$\begin{aligned} C_2 &:= C_2 - \theta_j C_2 x_j x_j^T C_2 \\ C_1 &:= C_1 + \frac{\theta_j}{\lambda_j}(C_2 x_j x_j^T C_0 + C_0 x_j x_j^T C_2) \\ C_0 &:= C_0 - \frac{\theta_j}{\lambda_j^2} C_0 x_j x_j^T C_0. \end{aligned}$$

where $\theta_j = (x_j^T C_2 x_j)^{-1}$;
if $\lambda_j = \alpha_j + i\beta_j$ *is complex and* $x_j = x_{jR} + ix_{jI}$, *then compute*

$$\begin{aligned} C_2 &:= C_2 - C_2 X_j \Theta_j X_j^T C_2 \\ C_1 &:= C_1 + C_2 X_j \Theta_j \Lambda_j^{-T} X_j^T C_0 + C_0 X_j \Lambda_j^{-1} \Theta_j^T X_j^T C_2 \\ C_0 &:= C_0 - C_0 X_j \Lambda_j^{-1} \Theta_j \Lambda_j^{-T} X_j^T C_0. \end{aligned}$$

where $\Lambda_j = \begin{bmatrix} \alpha_j & \beta_j \\ -\beta_j & \alpha_j \end{bmatrix}$, $X_j = [x_{jR}, x_{jI}]$ *and* $\Theta_j = (X_j^T C_2 X_j)^{-1}$.

(vii) Set $Q(\lambda) := \lambda^2 C_2 + \lambda C_1 + C_0$.
$m = 0,\ V = [],\ i = 2$.
While $(m \le m_{min})$ *do*
$V \leftarrow ModGS([V|v_i]),\ m = m+1,\ i = i+1,\ if\ v_i \in \mathbb{R}^n$;
$V \leftarrow ModGS([V|Re(v_i), Im(v_i)]),\ m = m+2,\ i = i+1,\ if\ v_i \in \mathbb{C}^n$.
End while m

End while j

Remark 3.1. (a) In step (ii) of Algorithm 3.1, since matrices H_0, H_1 and H_2 are all real, the Ritz values of $(\rho^2 H_2 + \rho H_1 + H_0)y = 0$ occur under closed complex conjugation and can be compute by standard QZ algorithm in real arithmetic.

(b) From Theorem 2.2 we see that the new deflated quadratic pencil given by (3.4) or (3.7) keeps the remaining eigenpairs, i.e., $\{(\lambda_i, x_i), i > 1\}$, invariant provided $\lambda_i \neq \lambda_1$. Therefore, the reduced QEP $\lambda^2 H_2 + \lambda H_1 + H_0$ in step (i) and the residual in step (v) can thus be computed by using the original data M, C and K.

(c) An approximate solution $\hat{t}$ $(\hat{t} \perp u)$ of the correction equation (3.10) can be solved by

$$\hat{t} = -M^{-1}\tilde{r} + \epsilon M^{-1} p \quad (\hat{t} \perp u), \tag{3.11}$$

where M is an approximate preconditioner of $Q(\rho_1)$ and

$$\epsilon = \frac{u^T M^{-1} \tilde{r}}{u^T M^{-1} p}. \tag{3.12}$$

In our numerical examples, M is chosen as a $SSOR(\omega)$ decomposition of $Q(\rho_1)$, i.e.,

$$M = (D_1 - \omega L_1)D_1^{-1}(D_1 - \omega U_1), \tag{3.13}$$

where $D_1 = \mathrm{diag}(Q(\rho_1)), L_1$ and U_1 are strictly lower and upper triangular of $Q(\rho_1)$, respectively.

(d) The quadratic Jacobi-Davidson method can also be applied to compute the interior eigenvalues of the spectrum of (1.1) without any inversion. Thus, a variant shift-target strategy can be designed to shift along the specified interval.

Based on a locking and restarting technique combined with Jacobi-Davidson developed in [14] for solving quadratic eigenvalue problems we summarize these approaches in the following algorithm.

Algorithm 3.2 ([14]). (*Quadratic Jacobi-Davidson Algorithm + Locking and Restarting*)

Input: *Matrices M, C, K as in (1.1). A target τ_0 with nonnegative imaginary part and a number ℓ of desired eigenpqairs nearest to τ_0. Positive integer numbers $\ell + 2 \le m_{min} \le m_{max}$ for the minimal and maximal dimensions of the search subspaces. Tolerance Tol for the stopping criterion. $\Lambda = \emptyset, V_0 = []$. Choose randomly a $n \times m_{min}$ real matrix $V \in \mathbb{R}^{n \times m_{min}}$.*

Output: *The ℓ desired eigenpairs $\{(\lambda_j, x_j)\}_{j=1}^{\ell}$ of*

$$Q(\lambda)x = (\lambda^2 M + \lambda C + K)x = 0,$$

associated with eigenvalues $\{\lambda_j\}_{j=1}^{\ell}$ that are nearest to the target τ_0

While $(j \le \ell)$ *do*

I. Start: let $m = m_{min}$. Orthonormalize V.

II. Repeat:

(i) Compute $H_2 \leftarrow V^T M V,\ H_1 \leftarrow V^T C V,\ H_0 \leftarrow V^T K V$.

(ii) Let $k = m_{min} - \sharp(\Lambda)$. *Compute* k *eigenpairs* $\{(\rho_i, y_i)\}_{i=1}^{k}$ *of*

$$(\rho^2 H_2 + \rho H_1 + H_0)y = 0,$$

where $\|y_i\|_2 = 1$, ρ_i *has nonnegative imaginary part and is not in* Λ *so that the eigenvalues* $\{\rho_i\}_{i=1}^{k}$ *are nearest to the target* τ_0 *satisfying*

$$|\rho_k - \tau_0| \geq \cdots \geq |\rho_1 - \tau_0|.$$

(iii) Compute $u \leftarrow Vy_1$, $p \leftarrow (2\rho_1 M + C)u$, $\{v_i \leftarrow Vy_i\}_{i=2}^{k}$.

(iv) Compute $r \leftarrow (\rho_1^2 M + \rho_1 C + K)u$.

(v) If $(\|r\|_2 < Tol)$, *then*

$\lambda_j = \rho_1$ $(Im(\rho_1) \geq 0)$, $x_j = u$, $\Lambda = \Lambda \cup \{\lambda_j\}$.

If λ_j *is real, then* $V_0 = [V_0|u]$, $j = j + 1$;

else $V_0 = [V_0|Re(u), Im(u)]$, $j = j + 2$.

Else

(v.1) Solve (approximately) a $\hat{t} \perp u$ *from*

$$(I - \frac{pu^H}{u^H p})Q(\rho_1)(I - uu^H)t = -r.$$

(v.2) Perform steps (v.2), (v.3) as in Algorithm 3.1.

Go to Repeat.

End if.

(vi) (Locking) Select a suitable target $\tau_0, m = \sharp(\Lambda)$, $V \leftarrow V_0$, $i = 2$.

While $(m \leq m_{min})$ *do*

$V \leftarrow ModGS([V|v_i])$, $m = m + 1$, $i = i + 1$, if $v_i \in \mathbb{R}^n$;

$V \leftarrow ModGS([V|Re(v_i), Im(v_i)])$, $m = m + 2$, $i = i + 1$, if $v_i \in \mathbb{C}^n$.

End while m

End while j

Remark 3.2. (a) In contrast to Algorithm 3.1, locking technique locks a desired eigenvalue by appending the associated eigenvector to the search subspace V. Thus, the reduced quadratic eigenvalue problem in step (ii) would yield a dummy(meaningless) Ritz value which is meaningless for the original $Q(\lambda)$. This dummy Ritz value sometimes might slow down the convergence of Jacobi-Davidson method.(See examples in Section 4).

(b) In Algorithm 3.1 the desired and computed eigenvalues are transformed to infinity which do not appear in the specified interval any more. Thus, we can either fix the original target or move the target to the new computed eigenvalue (which has been removed to infinity) and continue the Jacobi-Davidson iteration. In contrast to Algorithm 3.1, in the locking step (vi) of Algorithm 3.2 the selection of a new suitable target τ_0 is not so easy provided that the desired eigenvalues lie in a complex region.

4. Numerical Results

In this section we present some numerical results for testing algorithms developed in Section 3. All computation were done in FORTRAN90 on a Compaq DS20E workstation. We use the following abbreviation to denote algorithms proposed in Section 3.

- QJD_LR: Quadratic Jacobi-Davidson method + Locking and Restarting [14], given by Algorithm 3.2.
- QJD_NLD: Quadratic Jacobi-Davidson method + Non-equivalence Low-rank Deflation with a fixed target, given by Algorithm 3.1.
- QJD_NLD(q): Repeatedly select a new suitable target and compute q eigenpairs by QJD_NLD. (Deflate two or three eigenpairs which are closest to the target if necessary!)

Here in QJD_NLD(q), if the desired eigenvalues are required in a real interval, the selection strategy for the new targets can be arranged as follows. We begin with a target from the right most end of the interval, and then we move the target to the current qth eigenvalue (counted in a descent order) which has just been computed by QJD_NLD(q). To avoid the duplication, we can deflate the computed $(q-1)th$ and qth eigenpairs and continue the QJD_NLD(q).

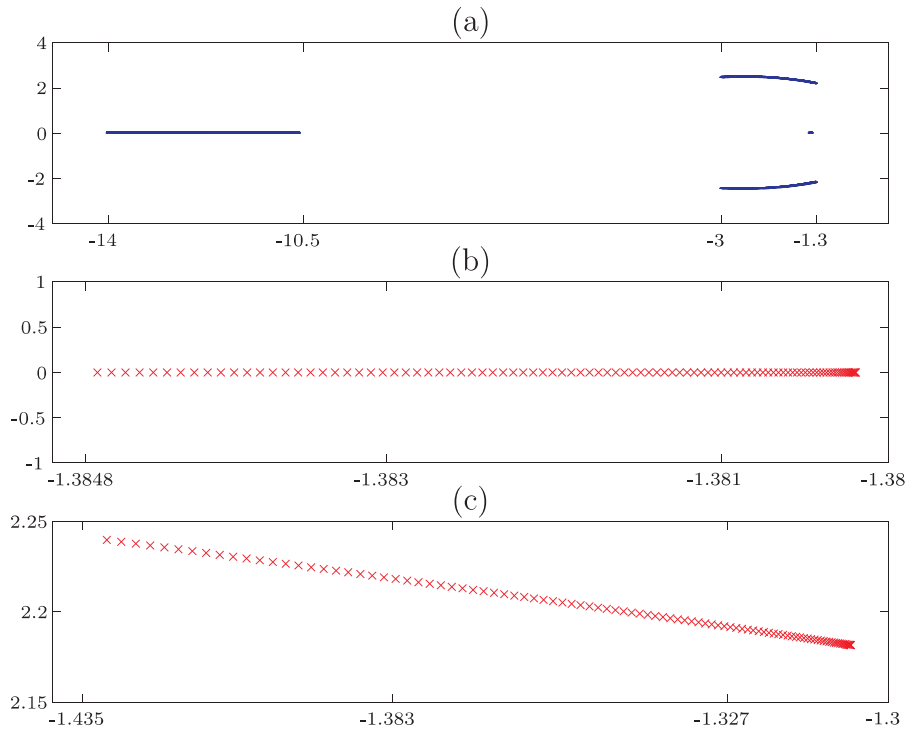

Figure 4.1: (a) The spectrum of $Q(\lambda) = \lambda^2 M + \lambda C + K$; (b) the 100 desired real eigenvalues; (c) the 100 desired complex eigenvalues

Example 4.1. A model quadratic eigenvalues problem [28]. Let

$$M = I_n,\ \ K = \kappa \mathrm{Trid}_n\{-1, 3, -1\},\ \ C = \gamma \mathrm{Trid}_n\{-1, diag\{4, 2, 4, \cdots, 2, 4\}, -1\},$$

where $n = 1000, \gamma = 3.0$ and $\kappa = 5.0$. Here $\mathrm{Trid}_n\{s, t, r\}$ denotes a tridiagonal matrix with sub-diagonal, diagonal and super-diagonal elements s, t and r, respectively. We show in Figure 4.1(a), the spectrum of the quadratic eigenvalue problem $Q(\lambda) = \lambda^2 M + \lambda C + K$, and in Figure 4.1(b),(c), the 100 desired real and complex eigenvalues, respectively.

We first compute the 100 desired real eigenvalues which are closest to zero (see Fig.4.1(b)) by using QJD_NLD and QJD_LR algorithms with $m_{max} = 50$, respectively. The stop tolerance Tol is chosen to be 10^{-13}. The relaxation parameter ω for $SSOR(w)$ decomposition in (3.13) is chosen to be 1.7, which is optimal in average in this example. We show that numbers of iterations and residuals versus orders of computed eigenvalues from zero

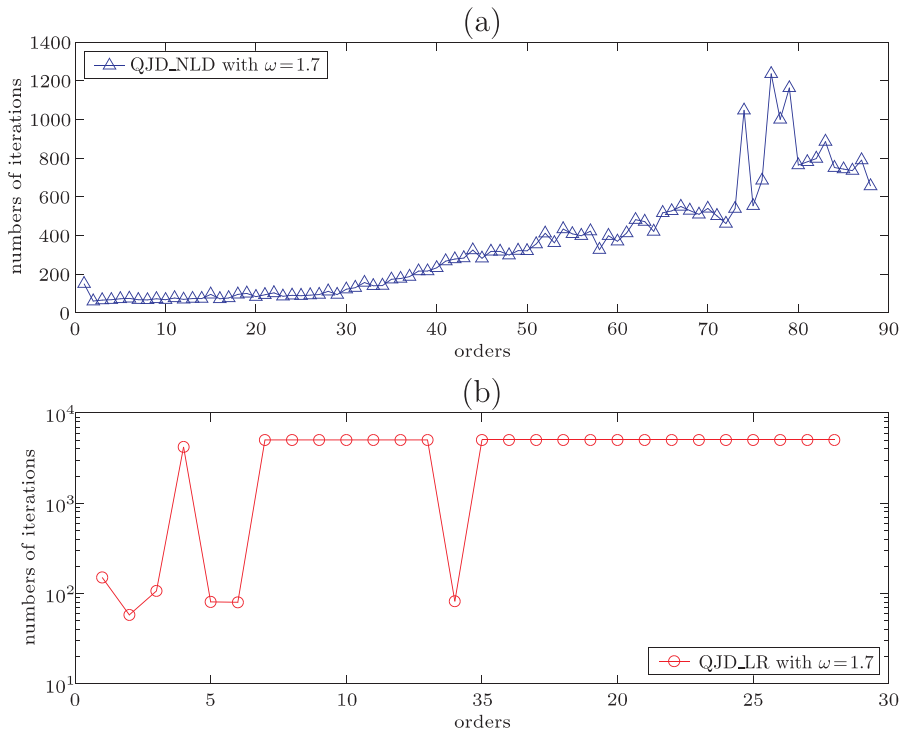

Figure 4.2: Numbers of iterations versus orders of computed real eigenvalues from zero toward the negative direction by (a) QJD_NLD, and (b) QJD_LR

toward the negative direction by QJD_NLD and QJD_LR in Figure 4.2 and Figure 4.3, respectively. In Figure 4.2(b) and Figure 4.3, respectively, we see that QJD_LR can compute only 6 desired eigenpairs, and the residuals of the other Ritz pairs oscillate between 10^{-4} and 10^{-10} repeatedly which cannot converge after 5000 iterations by QJD_LR. In Figure 4.4 we see that the differences between the computed eigenvalues by QJD_NLD and the eigenvalues computed by MATLAB in the same order are al less than 10^{-13}. This concludes that QJD_NLD algorithm never lost any desired eigenpairs for this example.

We now compute the desired real eigenvalues by QJD_NLD(10) with $\omega = 1.7$ starting with zero target. QJD_NLD(10) computes 10 eigenpairs from zero toward the negative direction with the current target. Then we move the target to the new computed tenth eigenvalue and continue applying QJD_NLD(10) to the new quadratic pencil by deflating the new computed ninth and tenth eigenpairs from the original matrices M, C and K. The

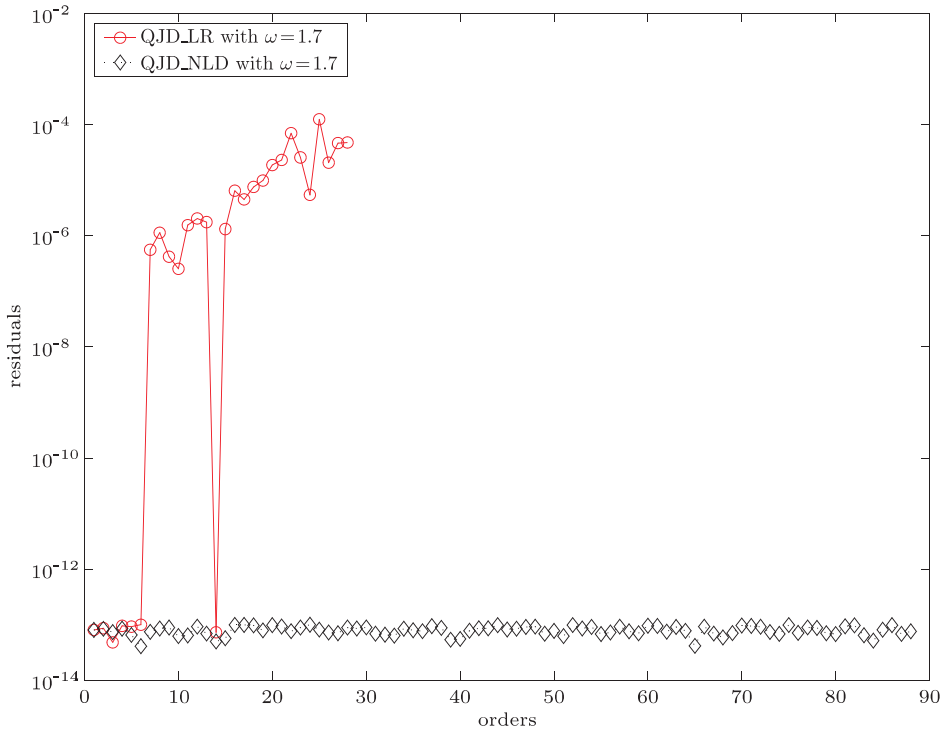

Figure 4.3: Residuals versus orders of the computed real eigenvalues from zero toward the negative direction by QJD_NLD and QJD_LR, respectively.

numbers of iterations and the CPU time versus orders of the computed real eigenvalues from the zero toward the negative direction by QJD_NLD and QJD_NLD(10), respectively, are shown in Figure 4.5(a) and (b). We see that the number of iterations of QJD_NLD(10) is larger than that of QJD_NLD, however, QJD_NLD(10) considerably saves computational cost.(See Figure 4.5(b)).

Since a shift-target strategy for finding complex eigenvalues is not so easy to design, we now use QJD_NLD to compute the 100 desired complex eigenvalues which are closest to $-1+2\imath$ (See Figure 4.1(c)). The fixed target is chosen by $-1+2\imath$. Figure 4.6 shows that numbers of iterations, CPU time and the difference between the computed eigenvalues by QJD_NLD and by MATLAB, respectively, versus orders in modulo of the computed complex eigenvalues by QJD_NLD. The performance of QJD_NLD for the computation of the desired complex eigenpairs works well.

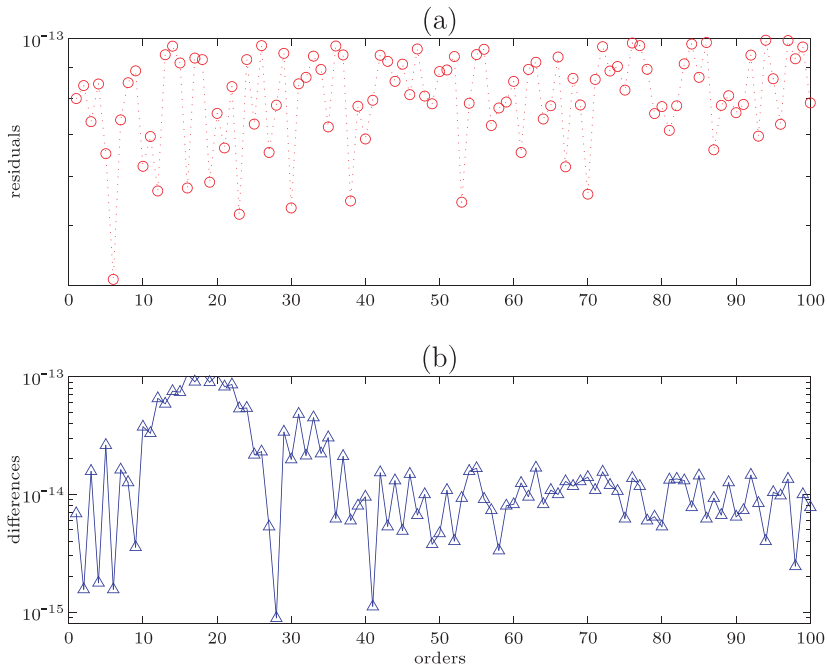

Figure 4.4: (a) Residuals, (b) the differences between the computed eigenvalues by QJD_NLD and by MATLAB, versus orders of the computed real eigenvalues by QJD_NLD

Example 4.2. We now construct a 12×12 artificial symmetric quadratic pencil $A(\lambda)$ with entries as follows,

$$(A(\lambda))_{i,i} = \begin{cases} (\lambda-1)(\lambda-1.5), & \text{if } i=1, \\ (\lambda-i)(\lambda-i-1), & \text{if } i=2,\ldots,10, \\ (1.5\lambda-2.5)(\lambda-3), & \text{if } i=11, \\ (\lambda-4)(\lambda-2), & \text{if } i=12, \end{cases}$$

$$(A(\lambda))_{i,i-1} = A(\lambda))_{i-1,i} = \begin{cases} 0, & \text{if } i=2,11, \\ \eta, & \text{if } i=3,\ldots,10, \\ (\lambda-1)(\lambda-2), & \text{if } i=12, \end{cases}$$

$$(A(\lambda))_{i,j} = \begin{cases} (\lambda-1)(\lambda-2), & \text{if } (i,j)=(11,1),(1,11), \\ \epsilon, & \text{if } (i,j)=(12,2),(2,12), \\ 0, & \text{otherwise, for } i+1>j \text{ or } i<j+1, \end{cases}$$

where $\epsilon = \eta = 10^{-9}$. The exact eigenvalues of $A(\lambda)$ are shown in Figure 4.7.

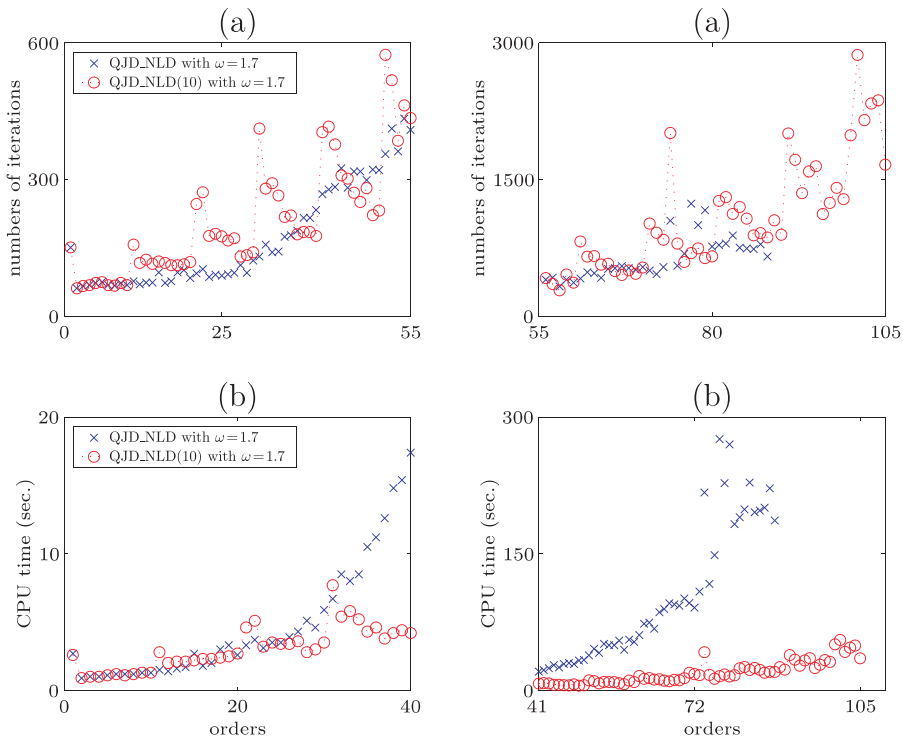

Figure 4.5: (a) The numbers of iterations, (b) CPU time, versus orders from 1-105 of the computed real eigenvalues by QJD_NLD and QJD_NLD(10), respectively.

Table 4.1: Iterations and residuals by QJD_NLD and QJD_LR, respectively.

	QJD_NLD		QJD_LR	
	iterations	residuals	iterations	residuals
λ_1	20	3.7e-14	20	3.7e-14
λ_2	7	1.2e-14	1436	2.8e-14
λ_3	3	1.0e-14	22	4.4e-14

In order to illustrate the convergence behavior of QJD_LR and QJD_NLD, we use these algorithms to compute the first three smallest eigenvalues λ_1, λ_2 and λ_3 of $A(\lambda)$. We choose the maximal number $m_{max} = 8$ for restarting, the stop tolerance $Tol = 5 \times 10^{-14}$ and the fixed target $\tau_0 = 0$.

In Table 4.1 we see that the QJD_NLD algorithm converges to the three desired eigenpairs of $A(\lambda)$ very fast within 10 iterations.

The QJD_LR algorithm also converges to the first and the third eigen-

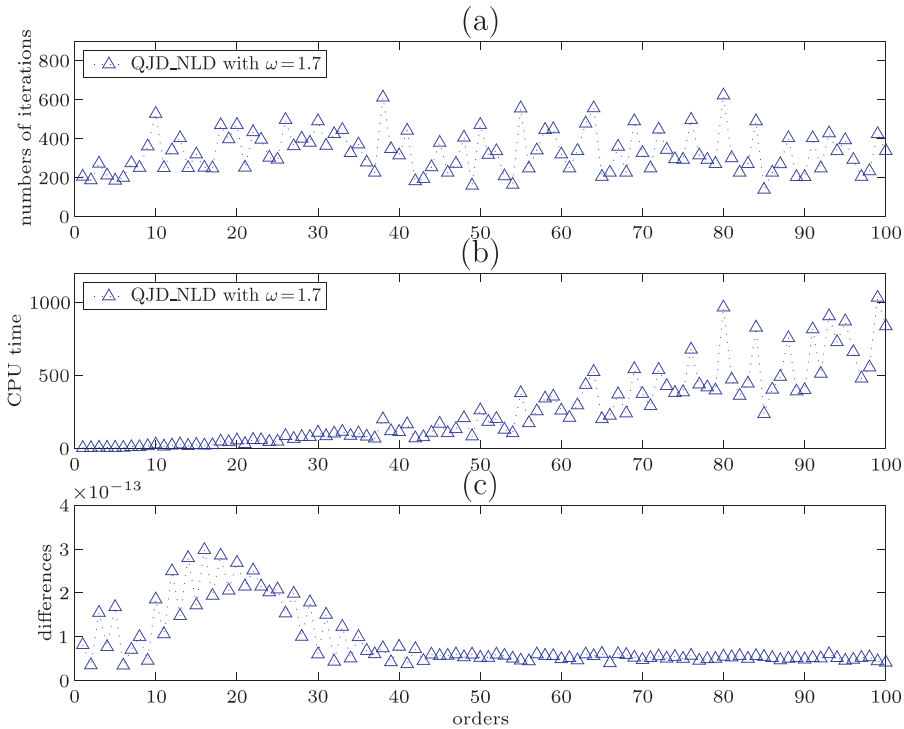

Figure 4.6: (a) Numbers of iterations, (b) CPU time, (c) the differences between the computed eigenvalues by QJD_NLD and by MATLAB, versus orders in moduls of the computed complex eigenvalues by QJD_NLD

pairs of $A(\lambda)$ very rapid, however, it needs 1436 iterations to converge to the second eigenpairs (See Table 4.1).

To look into the convergence behavior of QJD_LR in detail for the computation of λ_2, in Figure 4.8 we show that (a) and (b) the current Ritz values ρ_1 chosen by step (ii) of Algorithm 3.2; (c) and (d) the corresponding residuals, versus the iterations from 1 to 60 and 1380 to 1436, respectively. It is easily seen that the unit vector e_1 is the eigenvector of $A(\lambda)$ corresponding to $\lambda_1 = 1$ which will be locked in QJD_LR while finding the second smallest eigenvalue $\lambda_2 = 2$. We also see that the Ritz value $\rho_1 = 1.5$ computed by $e_1^T A(\rho)e_1 = 0$ is a dummy (meaningless) value of $A(\lambda)$. This artificial example is constructed so that the dummy value 1.5 always be chosen as a candidate closest to the target τ_0 unless the search subspace V in step (i) of Algorithm 3.2 contains some component in the direction e_{11}. Thus, if V has some component of e_{11}, then the value 1.5 is no longer a Ritz value of

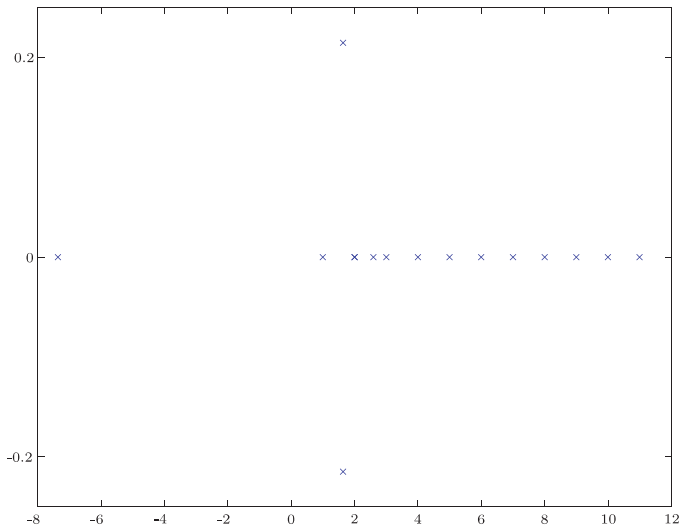

Figure 4.7: The spectrum of $A(\lambda)$

$V^T A(\lambda)V$ and a Ritz value $\rho \approx 2$ will be chosen as a candidate for finding λ_2. After this iteration, the Ritz pair will converges toward the desired eigenpairs, however, while performing restarting step, the search subspace V is reset by $V \approx [e_1, e_{12}]$, where e_{12} is an approximate eigenvector corresponding to λ_2, the dummy Ritz value $\rho_1 \approx 1.5$ is again to be chosen as a candidate for finding λ_2. The behavior of either choosing $\rho_1 \approx 1.5$ or 2 as a candidate and the corresponding residuals occur oscillatory in finding λ_2 by QJD_LR as shown in Figure 4.8 (a)-(d).

We construct an artificial example so that the dummy Ritz values influence and slow down the convergence of QJD_LR. In fact, the locking technique in [14] is developed based on the partial Schur form, however, a generalized Schur form does not always exist for a quadratic pencil. Hence, a mistaken choice of the dummy Ritz value cannot avoided in Algorithm 3.2.

In contrast to Algorithm 3.2, non-equivalence low-rank deflation in Algorithm 3.1 (QJD_NLD) removes the computed eigenvalue λ_1 to ∞, while keeping the other eigenpairs invariant. The computed eigenvector corresponding to λ_1 is not locked in V, so the dummy Ritz value 1.5 will not appear in step (ii) of Algorithm 3.1. Hence we have very satisfactory convergence using QJD_NLD as shown in Table 4.1.

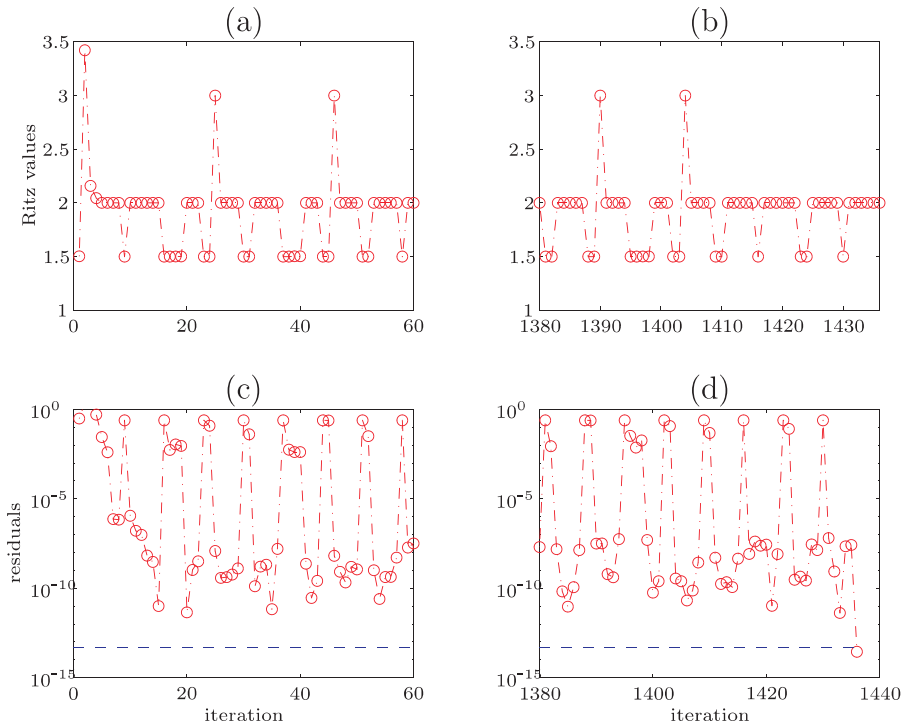

Figure 4.8: (a),(b) the current Ritz values ρ_1 chosen by step (ii) of algorithm 3.2; (c), (d) the corresponding residuals, versus the iterations from 1 to 60 and 1380 to 1436, respectively.

Example 4.3. Semiconductor quantum dot model with non-parabolic effective mass [8]

We consider a $2D$ time independent Schrödiger equation

$$\frac{\hbar^2}{2m_\ell(\lambda)}\left(\frac{\partial^2 F}{\partial x^2}+\frac{\partial^2 F}{\partial y^2}\right)+c_\ell F=\lambda F, \tag{4.1}$$

where $\hbar$ is the Plank constant, λ is the total energy and $F=F(x,y)$ is a wave function. The index ℓ depends on (x,y) is used to distinguish from the quantum dot (InAs, $\ell=1$) with a triangle shape and the matrix (GaAs, $\ell=2$). $c_1=0.0$ and $c_2=0.35$ denote the confinement potential in the ℓth region. The non-parabolic effective mass approximation satisfies equation

$$\frac{1}{m_\ell(\lambda)}=\frac{P_\ell^2}{\hbar^2}\left(\frac{2}{\lambda+g_\ell-c_\ell}+\frac{1}{\lambda+g_\ell-c_\ell+\delta_\ell}\right), \tag{4.2}$$

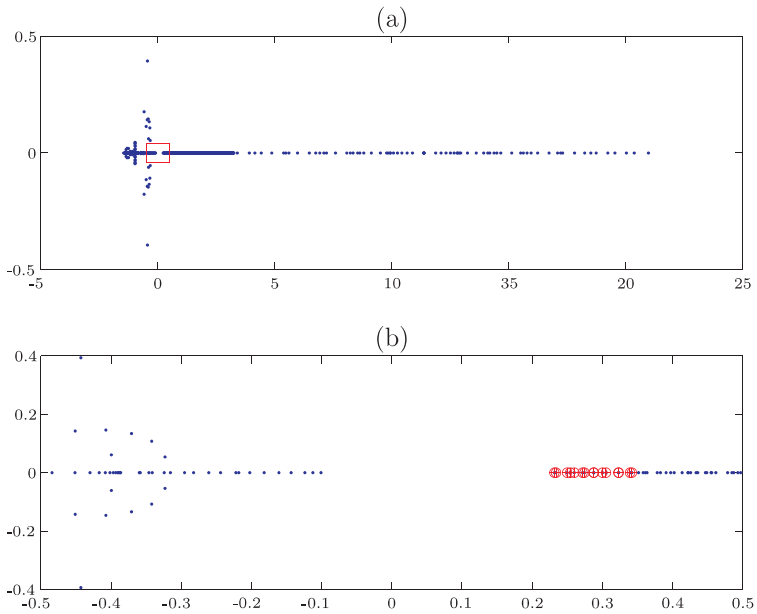

Figure 4.9: (a) The spectrum of eigenvalues of $B(\lambda)$. (b) Zoom in the rectangular box in (a).

where $P_1 = 0.2875, P_2 = 0.1993, g_1 = 0.235, g_2 1.59, \delta_1 = 0.81$ and $\delta_2 = 0.80$ denote the momentums, the energy gaps and the spin-orbit splitting in the ℓth region, respectively, in our numerical computation. The equation (4.1) is equipped with Dirichlet boundary condition and interface condition

$$\frac{-\hbar^2}{m_1(\lambda)}\frac{\partial F}{\partial \vec{n}}\,|_{I^+} = \frac{-\hbar^2}{m_2(\lambda)}\frac{\partial F}{\partial \vec{n}}\,|_{I^-}, \tag{4.3}$$

where I is the interface between the quantum dot and the matrix, and $\vec{n}$ is the normal unit vector of I.

Discretizing (4.1) and (4.3) by modified five-point finite difference, and multiplying the common denominators of (4.2), we simplify to get an approximate symmetric quadratic eigenvalue problem (see [8] for details)

$$B(\lambda)x = (\lambda^2 B_2 + \lambda B_1 + B_0)x = 0,$$

where B_0, B_1 are five-diagonal and B_2 is tridiagonal with B_0 and B_2 positive definite.

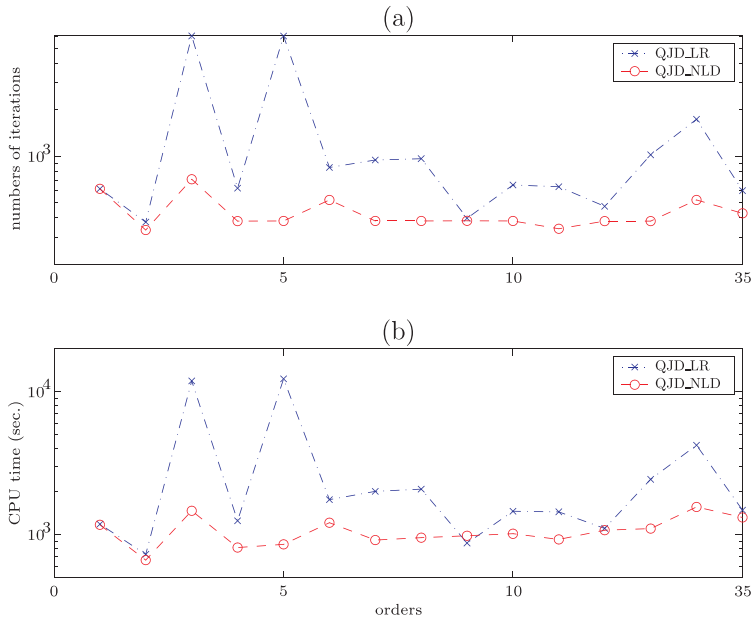

Figure 4.10: (a) The numbers of iterations, (b) CPU time, versus orders of the computed real positive eigenvalues by QJD_LR and QJD_NLD, respectively.

In Figure 4.9(a) we show the spectrum of eigenvalues of $B(\lambda)$ with the matrix size $n = 306081$. All eigenvalues are plotted in the complex plane with plus marks. The desired eigenvalues located within the interval $[0, 0.35]$ are emphasized by the mark $\oplus$ and zoomed in Figure 4.9(b). It is clear that the desired eigenvalues are embedded in the interior of the spectrum.

We now use QJD_LR and QJD_NLD to compute all discrete energy (eigenvalues) that are less than 0.35, of $B(\lambda)$ with matrix size $n = 306081$. The "*Tol*" is chosen by 5×10^{-13}. Figure 4.10 show all the numbers of iterations and the CPU time by QJD_LR and QJD_NLD, respectively.

References

1. E. Anderson, Z. Bai, C. Bischof, S. Blackford, J. Demmel, J. Dongarra, J. Du Croz, A. Greenbaum, S. Hammarling, A. McKenney and D. Sorensen. *LAPACK Users' Guide*. SIAM, Philadelphia, PA, third edition, 1999.

2. Z. Bai. Progress in the numerical solution of the nonsymmetric eigenvalue problem. *Num. Lin. Alg. Appl.*, **2**(1995), No. 3, 219-234.

3. Z. Bai, J. Demmel, J. Dongarra, A. Ruhe and H. van der Vorst. *Templates for the solution of algebraic eigenvalue problem: a practical guide*, SIAM, Philadelphia, PA, 2000.

4. B. N. Datta, S. Elhay and Y. M. Ram, Orthogonality and partial pole assigment for the symmetric definite quadratic pencil, *Linear Algebra Appl.*, **257**(1997), 29-48.

5. G. H. Golub and C. F. Van Loan, *Matrix Computations*, Johns Hopkins University Press, Baltimore, third edition, 1996.

6. J.-S. Guo, W.-W. Lin and C.-S. Wang. Numerical solutions for large sparse quadratic eigenvalue problems. *Linear Algebra Appl.*, **225**(1995), 57–89.

7. M. E. Hochstenbach and H. A. van der Vorst, Alternatives to the Rayleigh quotient for the quadratic eigenvalue problem. Technical Report 1212, Department of Mathematics, Univ. Utrecht, P.O. Box 80.010, NL-3508 TA Utrecht, The Netherlands, 2001.

8. T.-M. Hwang, W.-W. Lin, J.-L. Liu and W. Wang, Numerical computation of cubic eigenvalue problems for a semiconductor quantum dot model with non-parabolic effective mass approximation. Technical Report 2001-12, National Center for Theoretical Science, National Tsinghua University, Hsinchu 300, Taiwan, ROC, 2001.

9. T.-M. Hwang, W.-W. Lin and V. Mehrmann, Numerical solution of quadratic eigenvalue problems with structure preserving methods. *SIAM J. Sci. Comput.*, **24**(2003), 1283-1302.

10. R. B. Lehoucq, *Analysis and implementation of an implicitly restarted Arnoldi iteration*, PhD thesis, Rice University, Houston, TX, 1995.

11. R. B. Lehoucq and K. J. Maschhoff, Implementation of an implicitly restarted block Arnoldi method. Technical report, Argonne National Laboratory, Argonne, IL, 1997.

12. R. B. Lehoucq and D. C. Sorensen, Deflation techniques within an implicitly restarted Arnoldi iteration, *SIAM J. Matrix Anal. Appl.*, **17**(1996), 789-821.

13. R. B. Lehoucq, D. C. Sorensen and C. Yang, *ARPACK USERS GUIDE: Solution of large scale eigenvalue problems with implicitely restarted Arnoldi methods*, SIAM, Philadelphia, PA, 1998.

14. K. Meerbergen, Locking and restarting quadratic eigenvalue solvers. *SIAM J. Sci. Comput.*, **22**(2001), 1814-1839.

15. C. Mehl, *Compatible Lie and Jordan algebras and applications to structured matrices and pencils*, Dissertation, Fakultät für Mathematik, TU Chemnitz, 09107 Chemnitz (FRG), 1998.

16. Y. Saad, *Numerical Methods for Large Eigenvalue Problems*, Halsted Press, New York, 1992.

17. H. Schmitz, K. Volk and W. L. Wendland, On three-dimensional singularities of elastic fields near vertices, *Numer. Methods Partial Differ. Equations*, **9**(1993), 323-337.

18. H. R. Schwarz, *Methode der Finiten Elemente*, Teubner, Stuttgart, 1984.

19. B. Simon, J. Wu, O. Zienkiewicz and D. Paul, Evaluation of u-w and u-p finite element methods for the dynamic response of sturated porous media using one-dimensional models, *Internat. J. Numer. Anal. Methods Geomech.*, **10**(1986), 461-482.

20. G. L. G. Sleijpen, G. L. Booten, D. R. Fokkema and H. A. van der Vorst, Jacobi-Davidson type methods for generalized eigenproblems and polynomial eigenproblems, *BIT*, **36**(1996), 595–633.

21. G. L. G. Sleijpen and H. A. van der Vorst, A Jacobi-Davidson iteration method for linear eigenvalue problems, *SIAM J. Matrix Anal. Appl.*, **17**(1996), 401-425.

22. G. L. G. Sleijpen, H. A. van der Vorst and E. Meijerink, Efficient expansion of subspaces in the Jacobi-Davison method for standard and generalized eigenproblems, *Electron. Trans. Numer. Anal.*, **7**(1998), 75-89.

23. G. L. G. Sleijpen, H. A. van der Vorst and M. van Gijzen, Quadratic eigenproblems are no problem, *SIAM News*, **29**(1996), 8-9.

24. D.C. Sorensen, Implicit application of polynomial filters in a k-step Arnoldi method, *SIAM J. Matrix Anal. Appl.*, **13**, 357-385.

25. D. C. Sorensen, Deflation for implicitly restarted Arnoldi methods, Technical Report TR98-12, Department oc Computational and Applied Mathematics, Rice University, Houston, 1998.

26. G. W. Stewart and J.-G. Sun, *Matrix Perturbation Theory*, Academic Press, New York, 1990.

27. F. Tisseur, Backward error analysis of polynomial eigenvalue problems. *Linear Algebra Appl.*, **309**(2000), 339-361.

28. F. Tisseur and K. Meerbergen, The quadratic eigenvalue problem, *SIAM Rev.*, **43**(2001), 234-286.