A New Hybrid Method for Finding Eigenpairs of a Symmetric Quadratic Eigenvalue Problem in an Interval

Karabi Datta
&
Mohan Thapa

Northern Illinois University
Department of Mathematical Sciences
DeKalb, IL 60115  USA

First Conference of the Moroccan Applied Mathematical Society (MAMS)
06-08 February 2008, Rabat, Morocco.
Over View

I. Introduction

II. Parametrized Newton Method to Symmetric Quadratic Eigenvalue Problem

III. Convergence Criteria

IV. The New Hybrid Method

V. Results of Numerical Experiments

VI. Conclusions
I. Introduction

The symmetric quadratic eigenvalue problem

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

where $M$, $C$, and $K$ are given $n \times n$ matrices and $(\lambda, u)$ is an eigenpair.
Some Applications:

- **Vibration Analysis of Structural Systems**
  Undamped structural eigenvalue problem in industrial engineering

\[
(\lambda^2 Mu + Ku) = 0,
\]

In practice systems are subject to damping. Modern structures lead to non-classically damped eigenvalue problems

\[
\lambda^2 Mu + \lambda C u + Ku = 0.
\]
• Constrained least squares problem

\[ \min_{x^T x = \alpha^2} \{ x^T Ax - 2b^T x \} \]

where \( A = A^T \in \mathbb{R}^{n \times n}, b \in \mathbb{R}^n \).

The solution is \( x = (A - \lambda I)^{-1} b \), where \( \lambda \) is the smallest eigenvalue of

\[ (\lambda^2 I + 2\lambda A + (A^2 - \alpha^2 bb^T))y = 0, \]

• Eigenvalue assignment problem for quadratic matrix pencil
A Brief Review of the Existing Methods:

The Quadratic eigenvalue problem of the form
\((\lambda^2 M + \lambda C + K)x = 0\) is usually solved in two stages.

**Stage I.** Transform QEP into equivalent generalized Eigenvalue problem

\[ Ay = \lambda By \]

where

\[ A = \begin{pmatrix} -C & -K \\ I & O \end{pmatrix} \]

and

\[ B = \begin{pmatrix} M & O \\ O & I \end{pmatrix} \]

\((M\) is a non singular \(n \times n\) matrix).

**Stage II. Computing the Eigenpairs.**

Then find all the eigenpairs by using \(QZ\) algorithm if \(n\) is small and dense, or apply Krylov-subspace-based methods to find few eigenvalues of the \(QEP\).
Ib. OTHER METHODS

- Jacobi-Davidson Method for $QEP$:

  In this method, $QEP$ is not transformed into linear form; instead this method projects $QEP$ directly onto a properly chosen low-dimensional subspace where $QEP$ can be solved directly by a standard dense matrix technique.

- A recent second-order Arnoldi Method for the solution of the $QEP$ (Bai and Su (2005)).
Ic. Drawback of the Existing Methods:

• The coefficient matrices $M, C, K$ are symmetric positive definite but by the process of linearization, the transformed generalized eigenvalue problem becomes nonsymmetric, or symmetric indefinite. Subsequently the essential spectral properties of QEP are not guaranteed to be preserved.

• Also the generalized eigenvalue problem is twice the dimension of the original QEP.

• Successes of the Jacobi-Davidson Method strongly depends how to choose the initial eigenpair. Also this method targets one eigenpair at a time with local convergence verses Krylov Subspace in which a group of eigenvalues is approximated with global convergence.

• Second-order Arnoldi method does not give good approximation of eigenpair closer to the lower part of the spectrum. Also with this method it is not easy to find eigenvalues in a specific interval.
II. The Parametrized Newton Method to the Symmetric Quadratic Eigenvalue Problem

Define function: $f : \mathbb{R}^{n+1} \rightarrow \mathbb{R}^{n+1}$

$$f(\lambda, u) = \begin{pmatrix} Q(\lambda)u \\ u^T u - 1 \end{pmatrix},$$

where $Q(\lambda) = \lambda^2 M + \lambda C + K$, $M$, $C$, and $K \in \mathbb{R}^{n \times n}$ are symmetric positive definite matrices and $u \in \mathbb{R}^n$ and $\lambda \in \mathbb{R}$.

Jacobian matrix $J_f$ of $f$ which can be calculated as

$$J_f(\lambda, u) = \begin{pmatrix} Q(\lambda) & Q'(\lambda)u \\ 2u^T & 0 \end{pmatrix},$$

where $Q'(\lambda)= 2\lambda M + C$ is the derivative of the matrix polynomial $Q(\lambda)$. 
The Parametrized Newton Iterations for Symmetric Quadratic Pencil are:

\[
\begin{pmatrix}
x_{i+1} \\
\alpha_{i+1}
\end{pmatrix}
= \begin{pmatrix}
x_i \\
\alpha_i
\end{pmatrix} - \begin{pmatrix}
Q(\alpha_i) & Q'(\alpha_i)x_i \\
2x_i^T & 0
\end{pmatrix}^{-1} \begin{pmatrix}
Q(\alpha_i)x_i \\
x_i^Tx_i - 1
\end{pmatrix}.
\]

Now choose a parameter \( t > 0 \) and assume \( \alpha_i \neq 0 \) so that the method takes the form:

\[
\begin{pmatrix}
Q(\alpha_i) & Q'(\alpha_i)x_i \\
2x_i^T & 0
\end{pmatrix}
\begin{pmatrix}
x_{i+1} \\
\alpha_{i+1}
\end{pmatrix}
= \begin{pmatrix}
I & 0 \\
0 & t
\end{pmatrix} \begin{pmatrix}
0 & Q'(\alpha_i)x_i \\
x_i^T \frac{1}{\alpha_i}
\end{pmatrix} \begin{pmatrix}
x_i \\
\alpha_i
\end{pmatrix}.
\]
Parametrized Newton’s iteration for $Q(\lambda)$ now takes the form:

\begin{align*}
x_{i+1} &= \frac{1}{\hat{\beta}_i} Q^{-1}(\alpha_i) \cdot Q'(\alpha_i) x_i \quad (1) \\
\alpha_{i+1} &= \alpha_i - \frac{r_i}{\hat{\beta}_i} s \quad (2)
\end{align*}

\begin{align*}
\hat{\beta}_i &= ||Q^{-1}(\alpha_i)Q'(\alpha_i)x_i|| \\
\beta_i &= x_i^T Q^{-1}(\alpha_i)Q'(\alpha_i)x_i \\
r_i &= \frac{\beta_i}{\hat{\beta}_i}
\end{align*}

where we choose the value $s$ that gives the minimum residual
III. Convergence Criteria:

we define the residual at the \((i+1)^{th}\) step of Parametrized Newton’s Method by

\[
Res_{i+1} = Q(\alpha_{i+1})x_{i+1}. \tag{3}
\]

Using Parametrized Newton’s Iteration, we can then show that:

\[
||Res_{i+1}||^2 = \frac{1}{\hat{\beta}_i^2} [y_i^T y_i - 2\frac{r_{is}}{\hat{\beta}_i} y_i^T p_i - \frac{r_{is}^2}{\hat{\beta}_i^2} (2y_i^T z_i + p_i^T p_i) - 2\frac{r_{is}^3}{\hat{\beta}_i^3} p_i^T z_i + \frac{r_{is}^4}{\hat{\beta}_i^4} z_i^T z_i]. \tag{4}
\]

That is,

\[
||Res_{i+1}||^2 \leq \frac{1}{\hat{\beta}_i^2} [||y_i||^2 - 2\frac{r_{is}}{\hat{\beta}_i} y_i^T p_i + 2\frac{r_{is}^2}{\hat{\beta}_i^2} ||y_i|| ||z_i|| + \frac{r_{is}^3}{\hat{\beta}_i^3} ||p_i||^2 - 2\frac{r_{is}^3}{\hat{\beta}_i^3} p_i^T z_i + \frac{r_{is}^4}{\hat{\beta}_i^4} ||z_i||^2]
\]

where \(\hat{\beta}_i^2 = ||z_i||^2\), \(y_i = Q'(\alpha_i)x_i\),

\(z_i = Q^{-1}(\alpha_i)Q'(\alpha_i)x_i\), \(p_i = Q'(\alpha_i)z_i\),
IV. The New Hybrid Method:

1) a. we choose 3 sets of random eigenpairs \( (\alpha_i, v_i) \)
where \( \alpha_i \in [a, b] \), and the vectors \( v_i, i = 1, 2, 3 \)
are orthogonal to each other.

b. Use 3-iterations of Parametrized Newton’s method

2) Use these three eigenvectors to run the Jacobi-Davidson method.
New Hybrid Algorithm to Compute an Eigenpair of a Symmetric Quadratic Pencil in an Interval:

Define:

\[ Q(\lambda) = \lambda^2 M + \lambda C + K; \quad Q'(\lambda) = 2\lambda M + C \]

Where \( M, C, K \) are given

Let \([a, b]\) be the given interval.

Algorithm:

INPUT:

- The matrix \( M = I \in \mathbb{R}^{n \times n} \), \( C \), and \( K \in \mathbb{R}^{n \times n} \) symmetric positive definite matrices.
- Three real numbers \( \alpha_i, i=1, 2, 3 \) as initial approximations of an eigenvalues inside the interval \([a, b]\).
- An orthonormal matrix \( V = (v_1, v_2, v_3) \).

OUTPUT:
An approximate eigenpair of the QEP in the interval \([a, b]\).
Step 1: Find three approximate eigenpairs \((\alpha_i, v_i)\) using the Parametrized Newton’s method described in Section 2 (run only maximum of three iterations).

Step 2: Apply the Jacobi-Davidson method with the eigenvectors obtained in the Step 1 and a shift \(\alpha\) choosing it as one of the eigenvalues \(\alpha_i, i = 1, 2, 3\) appropriately (depending upon the location of the eigenvalue sought).

Step 3: Check if norm of the residual defined in equation (3) is less than a given tolerance. If so Stop. Otherwise, expand the search space \(V\) and return to Step 2.
V. Results of Numerical Experiments:

$M$ is identity matrix,
$C$, $K$ are arbitrary symmetric positive definite matrices
of order 500 and 800
Maximum number of iterations = 20
and tolerance = $10^{-4}$.

**Example 1**
Matrix size(n) = 500, Interval [41.5 43.5]
The approximate initial eigenvalue determined by the Parametrized Newton method = 42.0307903.
Exact eigenvalues in interval [41.5 43.5] are:
41.59431775969728, 41.62015325607620, 41.93211289355256, 43.00123828531239.

**TABLE 1: Convergence comparison between the Hybrid method and the Jacobi-Davidson method for Example 1**

<table>
<thead>
<tr>
<th>Methods</th>
<th>Residual</th>
<th>Iteration</th>
<th>Eigenvalue</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid</td>
<td>$1.9e^{-9}$</td>
<td>2</td>
<td>41.93211</td>
</tr>
<tr>
<td>JD</td>
<td>No convergence</td>
<td>20</td>
<td></td>
</tr>
</tbody>
</table>
Figure 1: Norm of log of Residual versus Iteration
Example 2
Matrix size $n = 800$, Interval $[70 \ 73]$
The approximate initial eigenvalue determined by the Parametrized Newton method $= 71.063630762458$.
Exact eigenvalues in interval $[70 \ 73]$ are: 
$71.48881531878268$, $72.89726841255406$.

TABLE 2: Convergence comparison between the Hybrid method and the Jacobi-Davidson method for Example 2

<table>
<thead>
<tr>
<th>Methods</th>
<th>Residual</th>
<th>Iteration</th>
<th>Eigenvalue</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid</td>
<td>$6.61e^{-6}$</td>
<td>1</td>
<td>71.4888153978</td>
</tr>
<tr>
<td>JD</td>
<td>No convergence</td>
<td>20</td>
<td></td>
</tr>
</tbody>
</table>
Figure 2: Norm of log of Residual *verses* Iteration
**Example 3**
Matrix size \(n = 800\), Interval \([60 \ 62]\)
The approximate initial eigenvalue determined by the Parametrized Newton method = 60.995819719.

Exact eigenvalues in interval \([60 \ 62]\) are:
60.38940860998, 60.95958197, 61.344186171, 61.796883006, 61.937923103.

**TABLE 3: Convergence comparison between the Hybrid method and the Jacobi-Davidson method for Example 3**

<table>
<thead>
<tr>
<th>Methods</th>
<th>Residual</th>
<th>Iteration</th>
<th>Eigenvalue</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hybrid</td>
<td>5.0e(-6)</td>
<td>2</td>
<td>60.38940860998</td>
</tr>
<tr>
<td>JD</td>
<td>No convergence</td>
<td>20</td>
<td></td>
</tr>
</tbody>
</table>
Figure 3: Norm of log of Residual versus Iteration
Conclusion:

• Numerical experimental results show that the hybrid method converges faster than the Jacobi-Davidson method alone for symmetric QEP; indeed, in some cases when the Jacobi-Davidson method did not converge at all, the new method worked quite well.

• The method is useful for many practical scientific and engineering applications.

• Studies on how to choose the parameter $s$ properly to guarantee or accelerate the convergence is currently underway and will be reported in a future paper.
References


THANK YOU