

Working Notes on the Fix-Heiberger reduction algorithm  
for solving the ill-conditioned generalized symmetric eigenvalue problem  
*prepared by C. Jiang and Z. Bai, April 21, 2015*<sup>1</sup>

**1. Introduction.** The generalized symmetric eigenvalue problem (GSEP) is of the form

$$Ax = \lambda Bx, \tag{1}$$

where  $A$  and  $B$  are  $n \times n$  real symmetric matrices, and  $B$  is positive definite. LAPACK routine `DSYSV` is a standard solver for the GSEP. In this notes, we describe a LAPACK-style routine for solving the GSEP, where  $B$  is positive semi-definite with respect to a prescribed threshold  $\varepsilon$ , where  $0 < \varepsilon \ll 1$ . In this case, the problem is called an *ill-conditioned* GSEP [2, 3].

With respect to a prescribed threshold  $\varepsilon$ , LAPACK-style routine `DSYGVIC` determines (a)  $A - \lambda B$  is regular and has  $k$   $\varepsilon$ -stable eigenvalues, where  $0 \leq k \leq n$ ; or (b)  $A - \lambda B$  is singular, namely  $\det(A - \lambda B) \equiv 0$  for any  $\lambda$ . It can be shown that the pencil  $A - \lambda B$  is singular if and only if  $\mathcal{N}(A) \cap \mathcal{N}(B) \neq \{0\}$ [1], where  $\mathcal{N}(Z)$  is the column null space of the matrix  $Z$ .

**2. New LAPACK-style routine DSYGVIC.**

The new routine `DSYGVIC` has the following calling sequence:

```
DSYGVIC( ITYPE, JOBZ, UPLO, N, A, LDA, B, LDB, ETOL, K, W, &
        WORK, LDWORK, WORK2, LWORK, IWORK, INFO )
```

Input to `DSYGVIC`:

**ITYPE:** Specifies the problem type to be solved: `ITYPE = 1` only.

**JOBZ:** = 'V': Compute eigenvalues and eigenvectors.

**UPLO:** = 'U': Upper triangles of  $A$  and  $B$  are stored;  
= 'L': Lower triangles of  $A$  and  $B$  are stored.

**N:** The order of the matrices  $A$  and  $B$ .  $N > 0$ .

**A, LDA:** The matrix  $A$  and the leading dimension of the array `A`.  $LDA \geq \max(1, N)$ .

**B, LDB:** The matrix  $B$  and the leading dimension of the array `B`.  $LDB \geq \max(1, N)$ .

**ETOL:** The parameter used to drop small eigenvalues of  $B$ .

**WORK, LDWORK:** The workspace matrix and the leading dimension of the array `WORK`.  $LDWORK \geq \max(1, N)$ .

**WORK2, LWORK:** The workspace array and its dimension.  $LWORK \geq \max(1, 3 * N + 1)$ . For optimal performance  $LWORK \geq 2 * N + (N + 1) * NB$  where `NB` is the optimal block size.

If `LWORK = -1`, then a workspace query is assumed; the routine only calculates the optimal size of the `WORK2` array, returns this value as the first entry of the `WORK2` array.

**IWORK:** The integer workspace array, dimension `N`.

Output from `DSYGVIC`:

**A:** Contains the eigenvectors matrix `X` in the first `K(1)` columns of `A`.

---

<sup>1</sup>Chengming Jiang and Zhaojun Bai, Department of Computer Science, University of California, Davis, CA 95616, cmjiang@ucdavis.edu and zbai@ucdavis.edu.

B: Contains the transformation matrix  $Q_1R_1Q_2Q_3$ , depending on the exit stage.

K: K(1) indicates the number of finite eigenvalues if INFO = 0; K(2) indicates the case number.

W: If K(1) > 0, W stores the K(1) eigenvalues.

INFO: = 0 then successful exit. If INFO =  $-i$ , the  $i$ -th argument had an illegal value.

**3. Algorithm.** LAPACK-style routine DSYGVIC is based on an algorithm first presented by Fix and Heiberger [2], also see [4, section 15.5]. The algorithm consists of the following three phases:

• **Phase 1.**

1. Compute the eigenvalue decomposition of  $B$ :

$$B^{(0)} = Q_1^T B Q_1 = D = \begin{matrix} n_1 & n_2 \\ \begin{bmatrix} D^{(0)} \\ E^{(0)} \end{bmatrix} \end{matrix}$$

where the diagonal entries of  $D^{(0)} = \text{diag}(d_{ii}^{(0)})$  are sorted in descending order and the diagonal elements of  $E^{(0)}$  are smaller than  $\varepsilon \cdot d_{11}^{(0)}$ .

2. *Early Exit:* If  $n_1 = 0$ , then  $B$  is a “zero” matrix with respect to  $\varepsilon$  and

(a) if  $\det(A) = 0$ , then  $A - \lambda B$  is singular. Program exits with output parameter (K(1),K(2)) = (-1, 1).

(b) if  $\det(A) \neq 0$ ,  $A - \lambda B$  is regular, but no finite eigenvalue. Program exits with output parameter (K(1),K(2)) = (0, 1).

3. Update  $A$ :

$$A^{(0)} = Q_1^T A Q_1$$

4. Set  $E^{(0)} = 0$ , and update  $A^{(0)}$  and  $B^{(0)}$ :

$$A^{(1)} = R_1^T A^{(0)} R_1 = \begin{matrix} n_1 & n_2 \\ \begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} \\ A_{12}^{(1)T} & A_{22}^{(1)} \end{bmatrix} \end{matrix} \quad \text{and} \quad B^{(1)} = R_1^T B^{(0)} R_1 = \begin{matrix} n_1 & n_2 \\ \begin{bmatrix} I & \\ & 0 \end{bmatrix} \end{matrix}$$

where

$$R_1 = \begin{matrix} n_1 & n_2 \\ \begin{bmatrix} (D^{(0)})^{-1/2} & \\ & I \end{bmatrix} \end{matrix}$$

5. *Early Exit:* If  $n_2 = 0$ , then  $B$  is a  $\varepsilon$ -well-conditioned matrix and  $B^{(1)} = I$ . There are  $n$   $\varepsilon$ -stable eigenvalues of the GSEP (1), which are the eigenvalues of  $A^{(1)}$ :

$$A^{(1)}U = U\Lambda. \tag{2}$$

The  $n$  eigenpairs of the GSEP (1) are  $(\Lambda, X = Q_1R_1U)$ . Program exits with output parameter (K(1),K(2)) = ( $n$ , 1).

• **Phase 2.**

1. Compute the eigenvalue decomposition of the (2,2) block  $A_{22}^{(1)}$  of  $A^{(1)}$ :

$$A_{22}^{(2)} = Q_{22}^{(2)T} A_{22}^{(1)} Q_{22}^{(2)} = \begin{matrix} n_3 & n_4 \\ n_3 & n_4 \end{matrix} \begin{bmatrix} D^{(2)} & \\ & E^{(2)} \end{bmatrix}$$

where the diagonal entries of  $D^{(2)} = \text{diag}(d_{ii}^{(2)})$  are in absolute-value-descending order and the diagonal elements of  $E^{(2)}$  are smaller than  $\varepsilon|d_{11}^{(2)}|$

2. *Early Exit*: If  $n_3 = 0$ , then  $A_{22}^{(1)} = 0$  and by setting  $E^{(2)} = 0$ , we have

$$A^{(1)} = \begin{matrix} n_1 & n_2 \\ n_2 & \end{matrix} \begin{bmatrix} A_{11}^{(1)} & A_{12}^{(1)} \\ A_{12}^{(1)T} & 0 \end{bmatrix} \quad \text{and} \quad B^{(1)} = \begin{matrix} n_1 & n_2 \\ n_2 & \end{matrix} \begin{bmatrix} I & \\ & 0 \end{bmatrix},$$

Then

- if  $n_1 < n_2$ ,  $A - \lambda B$  is singular. Program exits with output parameter  $(K(1), K(2)) = (-1, 2)$ .
- if  $n_1 \geq n_2$ , we reveal the rank of  $A_{12}^{(1)}$  by QR decomposition with pivoting:

$$A_{12}^{(1)} P_{12}^{(2)} = Q_{12}^{(2)} \begin{bmatrix} A_{13}^{(2)} \\ 0 \end{bmatrix}$$

where the diagonal entries in  $A_{13}^{(2)}$  are ordered in absolute-value-descending order.

- (a) If  $n_1 = n_2$  and  $A_{12}^{(1)}$  is rank deficient, then  $A - \lambda B$  is singular. Program exits with output parameter  $(K(1), K(2)) = (-1, 3)$ .
- (b) If  $n_1 = n_2$  and  $A_{12}^{(1)}$  is full rank, then  $A - \lambda B$  is regular, but no finite eigenvalues. Program exits with output parameter  $(K(1), K(2)) = (0, 2)$ .
- (c) If  $n_1 > n_2$  and  $A_{12}^{(1)}$  is rank deficient, then  $A - \lambda B$  is singular. Program exits with output parameter  $(K(1), K(2)) = (-1, 4)$ .
- (d) If  $n_1 > n_2$  and  $A_{12}^{(1)}$  is full column rank, then there are  $n_1 - n_2$   $\varepsilon$ -stable eigenvalues, which are the eigenvalues of

$$A^{(2)}U = B^{(2)}U\Lambda \tag{3}$$

where

$$A^{(2)} = Q_2^T A^{(1)} Q_2 = \begin{matrix} n_2 & n_1 - n_2 & n_2 \\ n_2 & n_1 - n_2 & n_2 \end{matrix} \begin{bmatrix} A_{11}^{(2)} & A_{12}^{(2)} & A_{13}^{(2)} \\ A_{12}^{(2)T} & A_{22}^{(2)} & \\ A_{13}^{(2)T} & & 0 \end{bmatrix},$$

$$B^{(2)} = Q_2^T B^{(1)} Q_2 = \begin{matrix} n_2 & n_1 - n_2 & n_2 \\ n_2 & n_1 - n_2 & n_2 \end{matrix} \begin{bmatrix} I & & \\ & I & \\ & & 0 \end{bmatrix}$$

and

$$Q_2 = \begin{matrix} n_1 & n_2 \\ n_2 & \end{matrix} \begin{bmatrix} Q_{12}^{(2)} & \\ & P_{12}^{(2)} \end{bmatrix}.$$

Let

$$U = \begin{matrix} & & n_1 - n_2 \\ & n_2 & \\ n_1 - n_2 & \begin{bmatrix} U_1 \\ U_2 \\ U_3 \end{bmatrix} & \\ & n_2 & \end{matrix}$$

Then the eigenvalue problem (3) are solved by

$$\begin{aligned} U_1 &= 0 \\ A_{22}^{(2)} U_2 &= U_2 \Lambda \\ U_3 &= -(A_{13}^{(2)})^{-1} A_{12}^{(2)} U_2 \end{aligned}$$

Consequently,  $n_1 - n_2$   $\varepsilon$ -stable eigenpairs of the original GSEP (1) are  $(\Lambda, X = Q_1 R_1 Q_2 U)$ . Program exits with output parameter  $(K(1), K(2)) = (n_1 - n_2, 2)$ .

3. Set  $E^{(2)} = 0$ , and update  $A^{(1)}$  and  $B^{(1)}$ :

$$A^{(2)} = Q_2^T A^{(1)} Q_2, \quad B^{(2)} = Q_2^T B^{(1)} Q_2$$

where

$$Q_2 = \begin{matrix} & n_1 & n_2 \\ n_1 & \begin{bmatrix} I \\ Q_{22}^{(2)} \end{bmatrix} \\ n_2 & \end{matrix}$$

4. *Early Exit*: If  $n_4 = 0$ , then  $A_{22}^{(1)}$  is a  $\varepsilon$ -well-conditioned matrix. We solve the eigenvalue problem

$$A^{(2)} U = B^{(2)} U \Lambda \tag{4}$$

where

$$A^{(2)} = \begin{matrix} & n_1 & n_2 \\ n_1 & \begin{bmatrix} A_{11}^{(2)} & A_{12}^{(2)} \\ A_{12}^{(2)T} & D^{(2)} \end{bmatrix} \\ n_2 & \end{matrix} \quad \text{and} \quad B^{(2)} = \begin{matrix} & n_1 & n_2 \\ n_1 & \begin{bmatrix} I \\ 0 \end{bmatrix} \\ n_2 & \end{matrix}$$

Let

$$U = \begin{matrix} & n_1 \\ n_1 & \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} \\ n_2 & \end{matrix}$$

The eigenvalue problem (4) becomes

$$\begin{aligned} (A_{11}^{(2)} - A_{12}^{(2)} (D^{(2)})^{-1} A_{12}^{(2)T}) U_1 &= U_1 \Lambda \\ U_2 &= -(D^{(2)})^{-1} (A_{12}^{(2)})^T U_1 \end{aligned}$$

Consequently,  $n_1$   $\varepsilon$ -stable eigenpairs of the original GSEP (1) are  $(\Lambda, X = Q_1 R_1 Q_2 U)$ . Program exits with output parameter  $(K(1), K(2)) = (n_1, 3)$ .

- **Phase 3.**

1. If  $n_4 \neq 0$ , then  $A_{22}^{(1)}$  is  $\varepsilon$ -ill-conditioned.  $A^{(2)}$  and  $B^{(2)}$  can be written as 3 by 3 blocks:

$$A^{(2)} = \begin{matrix} & \begin{matrix} n_1 & n_3 & n_4 \end{matrix} \\ \begin{matrix} n_1 \\ n_3 \\ n_4 \end{matrix} & \begin{bmatrix} A_{11}^{(2)} & A_{12}^{(2)} & A_{13}^{(2)} \\ A_{12}^{(2)T} & D^{(2)} & \\ A_{13}^{(2)T} & & 0 \end{bmatrix} \end{matrix} \quad \text{and} \quad B^{(2)} = \begin{matrix} & \begin{matrix} n_1 & n_3 & n_4 \end{matrix} \\ \begin{matrix} n_1 \\ n_3 \\ n_4 \end{matrix} & \begin{bmatrix} I & & \\ & 0 & \\ & & 0 \end{bmatrix} \end{matrix}$$

where  $n_3 + n_4 = n_2$ .

2. *Early Exit:* If  $n_1 < n_4$ , then  $A - \lambda B$  is singular. Program exits with output parameter  $(K(1), K(2)) = (-1, 5)$ .
3. When  $n_1 \geq n_4$ , we reveal the rank of  $A_{13}^{(2)}$  by QR decomposition with pivoting:

$$A_{13}^{(2)} P_{13}^{(3)} = Q_{13}^{(3)} R_{13}^{(3)}$$

where

$$R_{13}^{(3)} = \begin{matrix} & \begin{matrix} n_4 \end{matrix} \\ \begin{matrix} n_4 \\ n_5 \end{matrix} & \begin{bmatrix} A_{14}^{(3)} \\ 0 \end{bmatrix} \end{matrix}$$

4. *Early Exit:* (a) If  $n_1 = n_4$  and  $A_{13}^{(2)}$  is rank deficient, then  $A - \lambda B$  is singular. Program exits with output parameter  $(K(1), K(2)) = (-1, 6)$ .
- (b) If  $n_1 = n_4$  and  $A_{13}^{(2)}$  is full rank, then  $A - \lambda B$  is regular, but no finite eigenvalues. Program exits with output parameter  $(K(1), K(2)) = (0, 3)$ .
- (c) If  $n_1 > n_4$  and  $A_{13}^{(2)}$  is rank deficient,  $A - \lambda B$  is singular. Program exits with output parameter  $(K(1), K(2)) = (-1, 7)$ .
5. Update

$$A^{(3)} = Q_3^T A^{(2)} Q_3 \quad \text{and} \quad B^{(3)} = Q_3^T B^{(2)} Q_3$$

where

$$Q_3 = \begin{matrix} & \begin{matrix} n_1 & n_3 & n_4 \end{matrix} \\ \begin{matrix} n_1 \\ n_3 \\ n_4 \end{matrix} & \begin{bmatrix} Q_{13}^{(3)} & & \\ & I & \\ & & P_{13}^{(3)} \end{bmatrix} \end{matrix}$$

6. By the rank-revealing decomposition, matrices  $A^{(3)}$  and  $B^{(3)}$  can be written as  $4 \times 4$  blocks:

$$A^{(3)} = \begin{matrix} & \begin{matrix} n_4 & n_5 & n_3 & n_4 \end{matrix} \\ \begin{matrix} n_4 \\ n_5 \\ n_3 \\ n_4 \end{matrix} & \begin{bmatrix} A_{11}^{(3)} & A_{12}^{(3)} & A_{13}^{(3)} & A_{14}^{(3)} \\ (A_{12}^{(3)})^T & A_{22}^{(3)} & A_{23}^{(3)} & 0 \\ (A_{13}^{(3)})^T & (A_{23}^{(3)})^T & D^{(2)} & 0 \\ (A_{14}^{(3)})^T & 0 & 0 & 0 \end{bmatrix} \end{matrix} \quad \text{and} \quad B^{(3)} = \begin{matrix} & \begin{matrix} n_4 & n_5 & n_3 & n_4 \end{matrix} \\ \begin{matrix} n_4 \\ n_5 \\ n_3 \\ n_4 \end{matrix} & \begin{bmatrix} I & & & \\ & I & & \\ & & 0 & \\ & & & 0 \end{bmatrix},$$

where  $n_1 = n_4 + n_5$  and  $n_2 = n_3 + n_4$ . The  $\varepsilon$ -stable eigenpairs of the GSEP (1) are given by the finite eigenvalues of

$$A^{(3)}U = B^{(3)}U\Lambda \tag{5}$$

Let

$$U = \begin{matrix} & & & n_5 \\ & & & U_1 \\ n_4 & & & U_2 \\ & n_5 & & U_3 \\ & n_3 & & U_4 \\ & & n_4 & \end{matrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ U_4 \end{bmatrix}$$

then the eigenvalue problem (5) is equivalent to the following expressions:

$$\begin{aligned} U_1 &= 0 \\ (A_{22}^{(3)} - A_{23}^{(3)}(D^{(3)})^{-1}A_{23}^{(3)T})U_2 &= U_2\Lambda \\ U_3 &= -(D^{(2)})^{-1}A_{23}^{(3)T}U_2 \\ U_4 &= -(A_{14}^{(3)})^{-1}(A_{12}^{(3)}U_2 + A_{13}^{(3)}U_3) \end{aligned}$$

Consequently,  $n_5$   $\varepsilon$ -stable eigenpairs of the GSEP (1) are given by  $(\Lambda, X = Q_1R_1Q_2Q_3U)$ . Program exits with output parameter  $(K(1), K(2)) = (n_5, 4)$ .

**4. Numerical examples.** We design five test cases to illustrate major features of the routine **DSYGVIC**. For all these cases,

$$A = Q^T H Q \quad \text{and} \quad B = Q^T S Q$$

where  $Q$  is a random orthogonal matrix, and  $H$  and  $S$  are prescribed to be of certain structure for testing the different cases of the algorithm. Similar to the test of LAPACK routine **DSYGV**, the correctness of the routine **DSYGVIC** is measured by the following two residuals for computed eigenpairs  $(\hat{X}, \hat{\Lambda})$ :

$$\text{Res1} = \frac{\|A\hat{X} - B\hat{X}\hat{\Lambda}\|}{\|A\| \|\hat{X}\| + \|B\| \|\hat{X}\| \|\hat{\Lambda}\|} \quad \text{and} \quad \text{Res2} = \frac{\|\hat{X}^T B \hat{X} - I\|}{\|B\| \|\hat{X}\|}$$

1. **Test case 1.** Consider  $10 \times 10$  matrices  $A = Q^T H Q$  and  $B = Q^T S Q$ , where

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 2 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

and

$$S = \text{diag}[1, 2, 3, 2, 1, 1, 2, 3, 1, 2]$$

This is the case where  $B$  is positive definite and well-conditioned.

LAPACK routine **DSYGV** returns 10 eigenvalues with **INFO** = 0. New routine **DSYGVIC** with  $\varepsilon = 10^{-12}$  also returns 10 eigenvalues with **INFO** = 0. The computed eigenvalues agree to machine precision, with the comparable accuracy as shown in the following table:

	INFO	#eigvals	Res1	Res2
DSYGV	0	10	5.48e-17	2.41e-16
DSYGVIC	0	10	7.32e-17	2.38e-16

The output parameter  $(K(1), K(2)) = (10, 1)$  of DSYGVIC indicates that the matrix  $B$  is well-conditioned, and there are full set of finite eigenvalues of  $(A, B)$ . The original GSEP is reduced to the eigenvalue problem (2).

2. **Test case 2.** Consider  $8 \times 8$  matrices  $A = Q^T H Q$  and  $B = Q^T S Q$ , where

$$H = \begin{bmatrix} 6 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 5 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$S = \text{diag}[1, 1, 1, 1, \delta, \delta, \delta, \delta]$$

This is same test case used by Fix and Heiberger [2]. It is known that as  $\delta \rightarrow 0$ ,  $\lambda = 3, 4$  are the only stable eigenvalues.

Consider  $\delta = 10^{-15}$ , the following table shows the computed eigenvalues by LAPACK routine DSYGV and new routine DSYGVIC with the threshold  $\varepsilon = 10^{-12}$ .

$\lambda_i$	DSYGV	DSYGVIC
1	-0.3229260685047438e+08	<b>0.3000000000000001e+01</b>
2	-0.3107213627119420e+08	<b>0.3999999999999999e+01</b>
3	<b>0.2957918878610765e+01</b>	
4	<b>0.4150528124449937e+01</b>	
5	0.3107214204558684e+08	
6	0.3229261357421688e+08	
7	0.1004773743630529e+16	
8	0.2202090698823234e+16	

As we can see DSYGV returns all 8 eigenvalues including 6 unstable ones. For the two stable eigenvalues, there is significant loss of accuracy. In contrast, DSYGVIC only returns two stable eigenvalues to full machine precision.

3. **Test case 3.** Consider  $10 \times 10$  matrices  $A = Q^T H Q$  and  $B = Q^T S Q$ , where

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 2 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$S = \text{diag}[1, 2, 3, 2, 1, 1, 2\delta, 3\delta, \delta, 2\delta]$$

Note that  $B$  is very ill-conditioned for small  $\delta$ . Furthermore, the matrix  $H$  is designed such that the reduced matrix pair is of the form (3) with  $n_1 = 6$ ,  $n_2 = 4$  and  $n_3 = 0$ .

Consider  $\delta = 10^{-15}$ , LAPACK routine DSYGV treats  $B$  as a positive definite matrix and runs successfully with INFO = 0, but with significant loss of accuracy as shown in the following table. But DSYGVIC with the threshold  $\varepsilon = 10^{-12}$  computes two stable eigenvalues to machine precision.

	INFO	#eigvals	Res1	Res2
DSYGV	0	10	9.72e-11	5.08e-10
DSYGVIC	0	2	1.04e-16	8.20e-17

If  $\delta = 10^{-17}$ , LAPACK routine DSYGV detects  $B$  is not positive definite, and returns immediately with INFO = 17. In contrast, the new routine DSYGVIC with the threshold  $\varepsilon = 10^{-12}$  successfully completes the computation and reports there are two  $\varepsilon$ -stable eigenvalues with full machine accuracy:

	INFO	#eigvals	Res1	Res2
DSYGV	17	–	–	–
DSYGVIC	0	2	1.01e-16	1.12e-16

The output parameter (K(1),K(2))=(2,2) of DSYGVIC indicates that the program exits at the case that returns  $n_1 - n_2$  eigenvalues.

4. **Test case 4.** Consider  $10 \times 10$  matrices  $A = Q^T H Q$  and  $B = Q^T S Q$ , where

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 2 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

and

$$S = \text{diag}[1, 2, 3, 2, 1, 1, 2\delta, 3\delta, \delta, 2\delta],$$

where matrices  $H$  and  $S$  are designed such that the reduced eigenvalue problem is of the form (4) with  $n_1 = 6$ ,  $n_2 = 4$  and  $n_4 = 0$  as  $B$  becomes ill-conditioned.

Consider  $\delta = 10^{-15}$ , LAPACK routine DSYGV treats  $B$  as a positive definite matrix and runs successfully with INFO = 0, but with significant loss of accuracy as shown in the following table. But DSYGVIC with the threshold  $\varepsilon = 10^{-12}$  computes six stable eigenvalues to machine precision.

	INFO	#eigvals	Res1	Res2
DSYGV	0	10	5.50e-3	5.58e-10
DSYGVIC	0	6	2.45e-16	9.72e-16



If  $\delta = 10^{-17}$ , LAPACK routine DSYGV detects  $B$  is not positive definite, and returns immediately with `INFO = 17`. In contrast, the new routine DSYGVIC with  $\varepsilon = 10^{-12}$  returns 6  $\varepsilon$ -stable eigenvalues with the accuracy

	INFO	#eigvals	Res1	Res2
DSYGV	17	–	–	–
DSYGVIC	0	6	8.30e-17	2.02e-16

The output parameter  $(K(1), K(2)) = (6, 3)$  of DSYGVIC indicates that the program exits at the case that returns  $n_1$  eigenvalues.

5. **Test case 5.** Consider  $10 \times 10$  matrices  $A = Q^T H Q$  and  $B = Q^T S Q$ , where

$$H = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 2 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 2 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

and

$$S = \text{diag}[1, 2, 3, 2, 1, 1, 2\delta, 3\delta, \delta, 2\delta],$$

where  $H$  and  $S$  are designed such that the reduced eigenvalue problem is of the form (5) with  $n_1 = 6, n_2 = 4, n_3 = 2, n_4 = 2$  and  $n_5 = 4$  as  $\delta \rightarrow 0$ .

Consider  $\delta = 10^{-17}$ , LAPACK routine DSYGV detects  $B$  is not positive definite, and returns immediately with `INFO = 17`. In contrast, the new routine DSYGVIC with  $\varepsilon = 10^{-12}$  returns 4  $\varepsilon$ -stable eigenvalues with the accuracy

	INFO	#eigvals	Res1	Res2
DSYGV	17	–	–	–
DSYGVIC	0	4	8.49e-17	1.95e-16

The output parameter  $(K(1), K(2)) = (4, 4)$  of DSYGVIC indicates that the program exits at the case that returns  $n_5$  eigenvalues.

## 5. To do.

- CPU timing benchmark for large size  $n$ .
- Applications
- ...

## References

- [1] Z.-h. Cao. On a deflation method for the symmetric generalized eigenvalue problem. *Linear Algebra and its Applications*, 92:187–196, 1987.
- [2] G. Fix and R. Heiberger. An algorithm for the ill-conditioned generalized eigenvalue problem. *SIAM Journal on Numerical Analysis*, 9(1):78–88, 1972.
- [3] M. Jungun and R. Heiberger. The Fix-Heiberger procedure for solving the generalized ill-conditioned symmetric eigenvalue problem. *Inter. J. Quantum Chemistry*, 41(3):387–397, 1992.
- [4] B. Parlett. *The Symmetric Eigenvalue Problem*. Prentice Hall, Englewood Cliffs, NJ, 1980. SIAM Classics Edition 1998.