

Working Notes on the Fix-Heiberger reduction algorithm  
for solving the ill-conditioned generalized symmetric eigenvalue problem  
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**1. Introduction.** The generalized symmetric eigenvalue problem (GSEP) is of the form

$$Ax = \lambda Bx, \quad (1)$$

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  $\mathcal{N}(A) \cap \mathcal{N}(B) \neq \{0\}$ , where  $\mathcal{N}(Z)$  is the column null space of the matrix  $Z$  [1].

**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**.

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B: Contains the transformation matrix  $Q_1 R_1 Q_2 Q_3$ , 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)-ETOL-stable eigenvalues.

INFO: = 0 then successful exit.

= -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]. With some modification of the Fix-Heiberger algorithm, DSYGVIC consists of the following three phases:

- **Phase 1.**

1. Compute the eigenvalue decomposition of  $B$ :

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

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  $B^{(0)}$ :

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

where

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

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  $(\Lambda, X = Q_1 R_1 U)$ . 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  $A^{(1)}$ :

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

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

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

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

and

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

Let

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

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

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

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

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

Let

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

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

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

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:

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

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

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

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  $(\Lambda, X = Q_1 R_1 Q_2 Q_3 U)$ . 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 accuracy of computed eigenpairs  $(\hat{X}, \hat{\Lambda})$  is measured by the following two residuals:

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

**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).

**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 computes two stable eigenvalues to full machine precision.

**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.

**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.

**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.

- Theoretical analysis of the accuracy with respect to the threshold  $\varepsilon$
- CPU timing benchmark for large size  $n$ .
- Applications
- ...

## References

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