Symmetric definite generalized eigenvalue problem

- Symmetric definite generalized eigenvalue problem

$$Ax_i = \lambda_i B x_i$$

where

$$A^T = A \quad \text{and} \quad B^T = B > 0$$

- Eigen-decomposition

$$AX = BX\Lambda$$

where

$$\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$$
$$X = (x_1, x_2, \ldots, x_n)$$
$$X^T B X = I.$$

- Assume $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$

LAPACK solvers

- LAPACK routines `xSYGV`, `xSYGVD`, `xSYGVX` are based on the following algorithm (Wilkinson'65):
  1. compute the Cholesky factorization $B = GG^T$
  2. compute $C = G^{-1}AG^{-T}$
  3. compute symmetric eigen-decomposition $Q^T CQ = \Lambda$
  4. set $X = G^{-T}Q$
- `xSYGV[D,X]` could be *numerically unstable* if B is ill-conditioned:

  $$|\widehat{\lambda}_i - \lambda_i| \lesssim p(n)(\|B^{-1}\|_2\|A\|_2 + \text{cond}(B)|\widehat{\lambda}_i|) \cdot \epsilon$$

  and

  $$\theta(\widehat{x}_i, x_i) \lesssim p(n)\frac{\|B^{-1}\|_2\|A\|_2(\text{cond}(B))^{1/2} + \text{cond}(B)|\widehat{\lambda}_i|}{\text{specgap}_i} \cdot \epsilon$$
- User's choice between the inversion of ill-conditioned Cholesky decomposition and the QZ algorithm that destroys symmetry

A new LAPACK-style solver

- xSYGVIC: a LAPACK-style routine for computing ε-stable eigenpairs when $B^T = B \geq 0$ wrt a prescribed threshold ε.
- Implementation is based on Fix-Heiberger's algorithm, and organized in three phases.
- Given the threshold ε, xSYGVIC determines:
  1. $A - \lambda B$ is regular and has k $(0 \leq k \leq n)$ ε-stable eigenvalues **or**
  2. $A - \lambda B$ is singular.
- The new routine xSYGVIC has the following calling sequence:

```
xSYGVIC( ITYPE, JOBZ, UPLO, N, A, LDA, B, LDB, ETOL, &
    K, W, WORK, LDWORK, WORK2, LWORK2, IWORK, INFO )
```

xSYGVIC – Phase I

1. Compute the eigenvalue decomposition of B (xSYEV):

$$B^{(0)} = Q_1^T B Q_1 = D = \begin{array}{c} \\ n_1 \\ n_2 \end{array} \begin{array}{c} \begin{array}{cc} n_1 & n_2 \end{array} \\ \left[\begin{array}{cc} D^{(0)} & \\ & E^{(0)} \end{array} \right] \end{array},$$

   where diagonal entries of D: $d_{11} \geq d_{22} \geq \ldots \geq d_{nn}$, and elements of $E^{(0)}$ are smaller than $\varepsilon d_{11}^{(0)}$.

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

$$A^{(1)} = R_1^T Q_1^T A Q_1 R_1 = \begin{array}{c} \\ n_1 \\ n_2 \end{array} \begin{array}{c} \begin{array}{cc} n_1 & n_2 \end{array} \\ \left[\begin{array}{cc} A_{11}^{(1)} & A_{12}^{(1)} \\ A_{12}^{(1)T} & A_{22}^{(1)} \end{array} \right] \end{array}$$

   and

$$B^{(1)} = R_1^T B^{(0)} R_1 = \begin{array}{c} \\ n_1 \\ n_2 \end{array} \begin{array}{c} \begin{array}{cc} n_1 & n_2 \end{array} \\ \left[\begin{array}{cc} I & \\ & 0 \end{array} \right] \end{array},$$

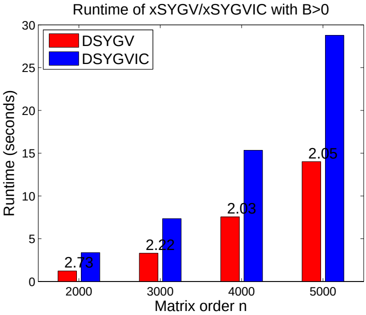
   where $R_1 = \text{diag}((D^{(0)})^{-1/2}, I)$

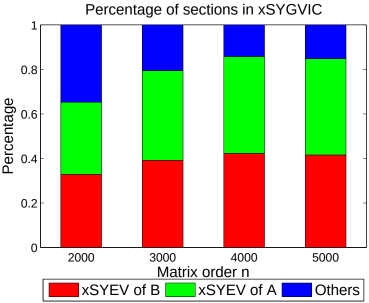
xSYGVIC – Phase I

3. *Early exit* B is ε-well-conditioned. $A - \lambda B$ is regular and has n ε-stable eigenpairs (Λ, X):
   - $A^{(1)}U = U\Lambda$ (xSYEV).
   - $X = Q_1 R_1 U$

$\texttt{xSYGVIC}$ – Phase I: performance profile

- Test matrices $A = Q_A D_A Q_A^T$ and $B = Q_B D_B Q_B^T$ where
  - Q_A, Q_B are random orthogonal matrices;
  - D_A is diagonal with $-1 < D_A(i,i) < 1, i = 1, \ldots, n$;
  - D_B is diagonal with $0 < \varepsilon < D_B(i,i) < 1, i = 1, \ldots, n$;
- 12-core on an Intel "Ivy Bridge" processor (Edison@NERSC)





xSYGVIC – Phase II

1. Compute the eigendecomposition of (2,2)-block $A_{22}^{(1)}$ of $A^{(1)}$ (xSYEV):

$$A_{22}^{(2)} = Q_{22}^{(2)T} A_{22}^{(1)} Q_{22}^{(2)} = \begin{array}{c} \\ n_3 \\ n_4 \end{array} \begin{array}{c} \begin{array}{cc} n_3 & n_4 \end{array} \\ \left[\begin{array}{cc} D^{(2)} & \\ & E^{(2)} \end{array} \right] \end{array}$$

   where eigenvalues are ordered such that $|d_{11}^{(2)}| \geq |d_{22}^{(2)}| \geq \cdots \geq |d_{n_2 n_2}^{(2)}|$, and elements of $E^{(2)}$ are smaller than $\varepsilon |d_{11}^{(2)}|$.

2. 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 $Q_2 = \text{diag}(I, Q_{22}^{(2)})$.

3. *Early exit* When $A_{22}^{(1)}$ is a ε-well-conditioned matrix. $A - \lambda B$ is regular and has n_1 ε-stable eigenpairs (Λ, X):
   - $A^{(2)} U = B^{(2)} U \Lambda$ (Schur complement and xSYEV)
   - $X = Q_1 R_1 Q_2 U$.

xSYGVIC – Phase II

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

where

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

. Let

$$U = \begin{array}{c} \\ n_1 \\ n_2 \end{array} \begin{array}{c} n_1 \\ \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} \end{array}$$

The eigenvalue problem (1) becomes

$$F^{(2)}U_1 = \left(A_{11}^{(2)} - A_{12}^{(2)}(D^{(2)})^{-1}A_{12}^{(2)T}\right)U_1 = U_1\Lambda \quad (\texttt{xSYEV})$$

$$U_2 = -(D^{(2)})^{-1}(A_{12}^{(2)})^T U_1$$

xSYGVIC – Phase II: performance profile

Accuracy:

1. If $B \geq 0$ has n_2 zero eigenvalues:
   - xSYGV stops, the Cholesky factorization of B could not be completed.
   - xSYGVIC successfully computes $n - n_2$ ε-stable eigenpairs.
2. If B has n_2 small eigenvalues about δ, both xSYGV and xSYGVIC "work", but produce different quality numerically.[1]
   - $n = 1000, n_2 = 100, \delta = 10^{-13}$ and $\varepsilon = 10^{-12}$.

	Res1	Res2
DSYGV	3.5e-8	1.7e-11
DSYGVIC	9.5e-15	7.1e-12

   - $n = 1000, n_2 = 100, \delta = 10^{-15}$ and $\varepsilon = 10^{-12}$.

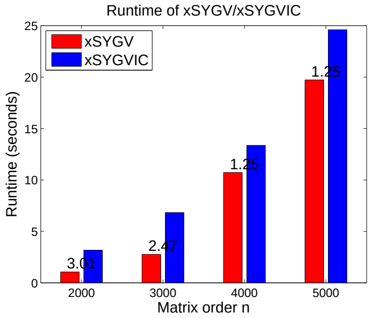
	Res1	Res2
DSYGV	3.6e-6	1.8e-10
DSYGVIC	1.3e-16	6.8e-14

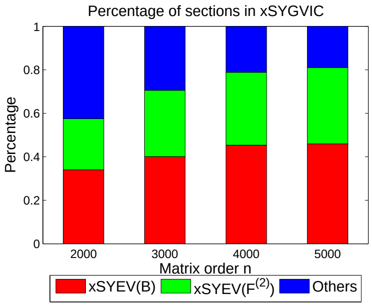
[1] Res1 $= \|A\widehat{X} - B\widehat{X}\widehat{\Lambda}\|_F/(n\|A\|_F\,\|\widehat{X}\|_F)$ and Res2 $= \|\widehat{X}^T B\widehat{X} - I\|_F/(\|B\|_F\,\|\widehat{X}\|_F^2)$.

xSYGVIC – Phase II: performance profile

Timing:

- Test matrices $A = Q_A D_A Q_A^T$ and $B = Q_B D_B Q_B^T$ where
  - Q_A, Q_B are random orthogonal matrices;
  - D_A is diagonal with $-1 < D_A(i,i) < 1, i = 1, \ldots, n$;
  - D_B is diagonal with $0 < D_B(i,i) < 1, i = 1, \ldots, n$ and n_2/n $D_B(i,i) < \varepsilon$.
- 12-core on an Intel "Ivy Bridge" processor (Edison@NERSC)

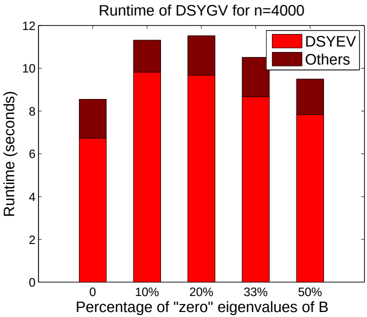




xSYGVIC – Phase II: performance profile

Why the extra cost ratio is lower?

CPU time of xSYGV varies due to the percentage of “zero” eigenvalues of B. For example, for $n = 4000$ on a 12-core processor execution:



xSYGVIC – Phase III

1. $A^{(2)}$ and $B^{(2)}$ can be written as 3 by 3 blocks:

$$A^{(2)} = \begin{array}{c} \\ n_1 \\ n_3 \\ n_4 \end{array} \begin{array}{c} \begin{array}{ccc} n_1 & n_3 & n_4 \end{array} \\ \left[\begin{array}{ccc} A_{11}^{(2)} & A_{12}^{(2)} & A_{13}^{(2)} \\ A_{12}^{(2)T} & D^{(2)} & \\ A_{13}^{(2)T} & & 0 \end{array} \right] \end{array} \quad \text{and} \quad B^{(2)} = \begin{array}{c} \\ n_1 \\ n_3 \\ n_4 \end{array} \begin{array}{c} \begin{array}{ccc} n_1 & n_3 & n_4 \end{array} \\ \left[\begin{array}{ccc} I & & \\ & 0 & \\ & & 0 \end{array} \right] \end{array}$$

where $n_3 + n_4 = n_2$.

2. 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

$$R_{13}^{(3)} = \begin{array}{c} \\ n_4 \\ n_5 \end{array} \begin{array}{c} n_4 \\ \left[\begin{array}{c} A_{14}^{(3)} \\ 0 \end{array} \right] \end{array}$$

xSYGVIC – Phase III

3. Final exit When $n_1 > n_4$ and $A_{13}^{(2)}$ is full rank,[2] then $A - \lambda B$ is regular and has $n_1 - n_4$ ε-stable eigenpairs (Λ, X):
   - $A^{(3)}U = B^{(3)}U\Lambda$
   - $X = Q_1 R_1 Q_2 Q_3 U$.

[2]All the other cases either lead $A - \lambda B$ to be "singular" or "regular but no finite eigenvalues".

xSYGVIC – Phase III

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

- Update

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

where

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

- Write $A^{(3)}$ and $B^{(3)}$ as 4×4 blocks:

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

where $n_1 = n_4 + n_5$ and $n_2 = n_3 + n_4$.

xSYGVIC – Phase III

- Let

$$U = \begin{array}{c} \\ n_4 \\ n_5 \\ n_3 \\ n_4 \end{array} \begin{array}{c} n_5 \\ \left[\begin{array}{c} U_1 \\ U_2 \\ U_3 \\ U_4 \end{array} \right] \end{array}$$

then the eigenvalue problem (2) becomes:

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

xSYGVIC – Phase III: performance profile

Test case (Fix-Heiberger'72)

1. Consider 8×8 matrices:

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

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

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

As $\delta \to 0$, $\lambda = 3, 4$ are the only stable eigenvalues of $A - \lambda B$.

xSYGVIC – Phase III: performance profile

2. The computed eigenvalues when $\delta = 10^{-15}$:

λ_i	eig(A,B,'chol')	DSYGV	DSYGVIC($\varepsilon = 10^{-12}$)
1	-3.334340289520080e+07	-0.3229260685047438e+08	**0.3000000000000001e+01**
2	-3.138309114827999e+07	-0.3107213627119420e+08	**0.3999999999999999e+01**
3	**2.999999998949329e+00**	**0.2957918878610765e+01**	
4	**3.999999999513074e+00**	**0.4150528124449937e+01**	
5	3.138309673669569e+07	0.3107214204558684e+08	
6	3.334340856015300e+07	0.3229261357421688e+08	
7	1.077763236890488e+15	0.1004773743630529e+16	
8	2.468473375420724e+15	0.2202090698823234e+16	