Solving Symmetric Semi-definite (ill-conditioned) Generalized Eigenvalue Problems

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Symmetric definite generalized eigenvalue problem

- Symmetric definite generalized eigenvalue problem

  $$Ax = \lambda Bx$$

  where

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

- Eigen-decomposition

  $$AX = BX\Lambda$$

  where

  $$\begin{aligned} \Lambda &= \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) \\ X &= (x_1, x_2, \ldots, x_n) \\ X^T BX &= I. \end{aligned}$$

- 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 $Q^TCQ = \Lambda$
  4. set $X = G^{-T}Q$
- `xSYGV[D,X]` could be *numerically unstable* if B is ill-conditioned:

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

  and

$$\theta(\widehat{x}_i, x_i) \lesssim p(n)\frac{\|B^{-1}\|_2\|A\|_2(\mathrm{cond}(B))^{1/2} + \mathrm{cond}(B)|\widehat{\lambda}_i|}{\mathrm{specgap}_i} \cdot \epsilon$$

- User's choice between the inversion of ill-conditioned Cholesky decomposition and the QZ algorithm that destroys symmetry

Algorithms to address the ill-conditioning

1. Fix-Heiberger'72 (Parlett'80): explicit reduction
2. Chang-Chung Chang'74: SQZ method (QZ by Moler and Stewart'73)
3. Bunse-Gerstner'84: MDR method
4. Chandrasekaran'00: "proper pivoting scheme"
5. Davies-Higham-Tisseur'01: Cholesky+Jacobi
6. Working notes by Kahan'11 and Moler'14

This talk

Three approaches:

1. A LAPACK-style implementation of Fix-Heiberger algorithm
2. An algebraic reformulation
3. Locally accelerated block preconditioned steepest descent (LABPSD)

This talk

Three approaches:

1. A LAPACK-style implementation of Fix-Heiberger algorithm
   Status: beta-release
2. An algebraic reformulation
   Status: completed basic theory and proof-of-concept
3. Locally accelerated block preconditioned steepest descent (LABPSD)
   Status: published two manuscripts, software to be released

A LAPACK-style implementation of Fix-Heiberger algorithm

(with C. Jiang)

A LAPACK-style solver

- xSYGVIC: computes 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):

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

   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 $B^{(0)}$:

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

   and

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

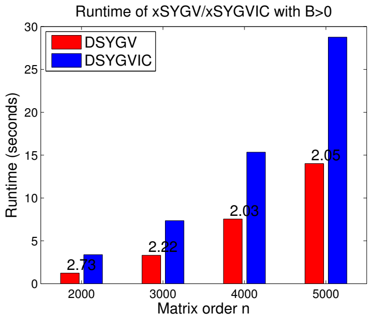
   where $R_1 = \text{diag}((D^{(0)})^{-1/2}, I)$

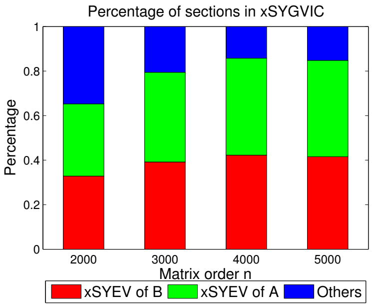
xSYGVIC – Phase I

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

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):

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

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

3. $\boxed{\textit{Early exit}}$ 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 (backup)

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

where

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

. Let

$$U = \begin{array}{cc} & n_1 \\ \begin{array}{c} n_1 \\ n_2 \end{array} & \left[\begin{array}{c} U_1 \\ U_2 \end{array}\right] \end{array}$$

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 $\varepsilon = 10^{-12}$.

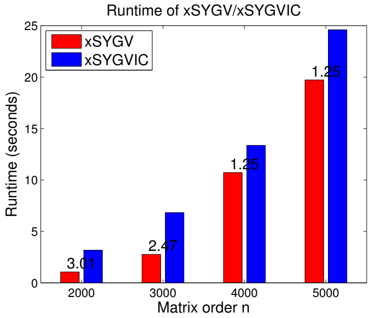
	Res1	Res2
DSYGV	3.6e-6	1.8e-10
DSYGVIC	1.3e-16	6.8e-14

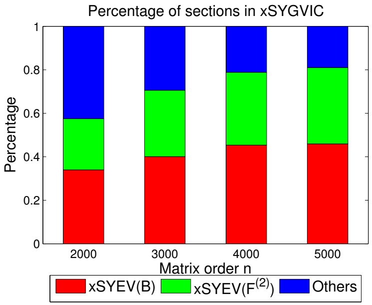
[1] Res1 $= \|A\widehat{X} - B\widehat{X}\widehat{\Lambda}\|_F/(n\|A\|_F\,\|\widehat{X}\|_F)$ and Res2 $= \|\widehat{X}^T B\widehat{X} - I\|_F/(\|B\|_F\,\|\widehat{X}\|_F^2)$.

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)

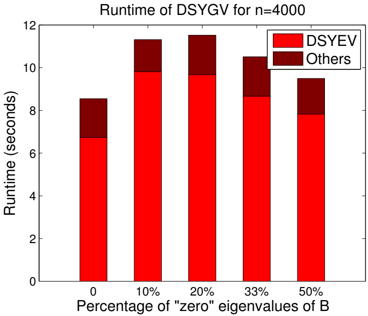




xSYGVIC – Phase II: performance profile

Why is the overhead ratio of xSYGVIC lower?

- Performance of xSYGV varies depending on 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:

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

   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

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

xSYGVIC – Phase III

3. $\boxed{\textit{Final exit}}$ 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 (backup)

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

- Update

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

where

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

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

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

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

xSYGVIC – Phase III (backup)

- Let

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

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	

An algebraic reformulation
(with H. Xie)

Symmetric semi-definite pencil

Symmetric semi-definite pencil:

$$A - \lambda B, \quad \text{with } A^T = A \text{ and } B^T = B \geq 0$$

Symmetric semi-definite pencil

Canonical form. There exists a nonsingular matrix $W \in \mathrm{R}^{n\times n}$ such that

$$W^TAW = \begin{array}{c} \\ 2n_1 \\ r \\ n_2 \\ s \end{array} \begin{array}{c} \begin{array}{cccc} 2n_1 & r & n_2 & s \end{array} \\ \left[\begin{array}{cccc} \Lambda_1 & & & \\ & \Lambda_2 & & \\ & & \Lambda_3 & \\ & & & 0 \end{array}\right] \end{array} \text{ and } W^TBW = \begin{array}{c} \\ 2n_1 \\ r \\ n_2 \\ s \end{array} \begin{array}{c} \begin{array}{cccc} 2n_1 & r & n_2 & s \end{array} \\ \left[\begin{array}{cccc} \Omega_1 & & & \\ & I & & \\ & & 0 & \\ & & & 0 \end{array}\right] \end{array}$$

where

$$\Lambda_1 = I_{n_1} \otimes K, \Lambda_2 = \mathrm{diag}(\lambda_i), \Lambda_3 = \mathrm{diag}(\pm 1), \Omega_1 = I_{n_1} \otimes T$$

and

$$K = \left[\begin{array}{cc} 0 & 1 \\ 1 & 0 \end{array}\right], \quad T = \left[\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array}\right]$$

Algebraic reformulation

Theorem [Xie and B.'16]. Suppose that the symmetric semi-definite pencil $A - \lambda B$ is regular and simultaneously diagonalizable with a congruence transformation. Given a symmetric positive definite matrix $H \in \mathrm{R}^{k\times k}$ and $\mu \in \mathrm{R}$, let us define

$$\widetilde{A} = A + \mu(AZ)H(AZ)^T, \quad \widetilde{B} = B + (AZ)H(AZ)^T,$$

where $Z \in \mathrm{R}^{n\times k}$ spans the nullspace of B. Then[3]

(1) The pencil $\widetilde{A} - \lambda \widetilde{B}$ is symmetric definite,

(2) $\lambda(\widetilde{A}, \widetilde{B}) = \lambda_{\mathrm{f}}(A, B) \cup \lambda(\mu H + (Z^T AZ)^{-1}, H)$

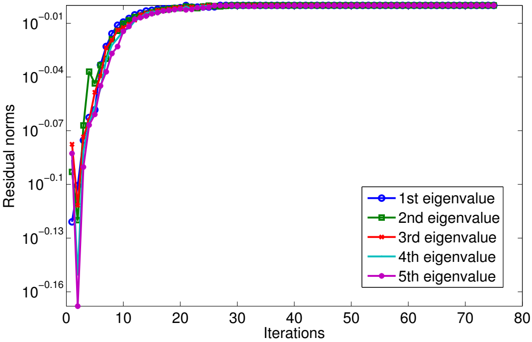
By appropriately chosen H and μ, one can compute the k smallest (finite) eigenvalues of $A - \lambda B$ directly, say by LOBPCG.

[3] Notations: $\lambda(A, B)$ denotes the set of eigenvalues of a pencil $A - \lambda B$. $\lambda_{\mathrm{f}}(A, B)$ denotes the set of all finite eigenvalues of $A - \lambda B$.

Algebraic reformulation

A test case from structure dynamics

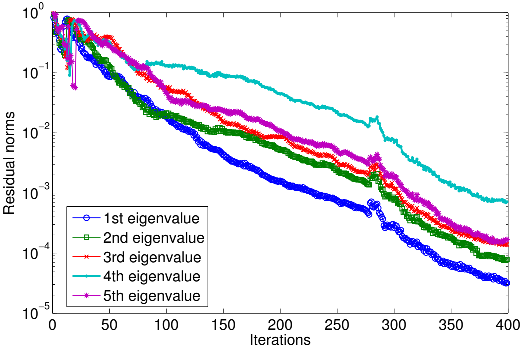
LOBPCG:



Algebraic reformulation

A test case from structure dynamics

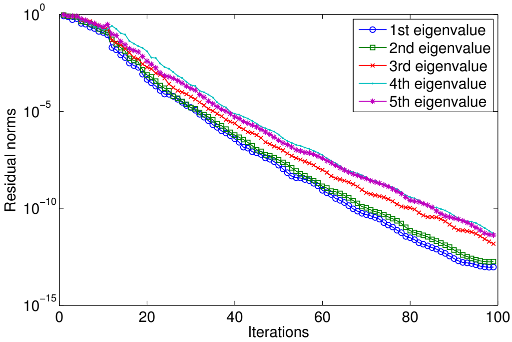
Algebraic reformulation + LOBPCG without preconditioning



Algebraic reformulation

A test case from structure dynamics

Algebraic reformulation + LOBPCG with preconditioning



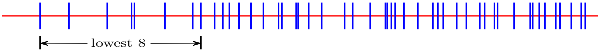
A locally accelerated BPSD (LABPSD)

Ill-conditioned GSEP

GSEP:

$$Hu_i = \lambda_i S u_i$$

1. Matrices H and S are ill-conditioned
   e.g., $\mathrm{cond}(H), \mathrm{cond}(S) = \mathcal{O}(10^{10})$
2. Share a *near-nullspace* span$\{V\}$
   e.g., $\|HV\| = \|SV\| = \mathcal{O}(10^{-4})$
3. No obvious spectrum gap between eigenvalues of interest and the rest
   e.g.,



PSD*id*

- **PSD***ed*: Preconditioned Steepest Descent with implicit deflation
- Assume the first $i-1$ eigenpairs $(\lambda_1, u_1), \ldots, (\lambda_{i-1}, u_{i-1})$ computed, and denote $U_{i-1} = [u_1, u_2, \ldots, u_{i-1}]$.
- **PSD***id* computes the i-th eigenpair (λ_i, u_i)

0 initialize $(\lambda_{i;0}, u_{i;0})$
1 for $j = 0, 1, \ldots$ until convergence
2 compute $r_{i;j} = H u_{i;j} - \lambda_{i;j} S u_{i;j}$
3 precondition $p_{i;j} = -K_{i;j} r_{i;j}$
4 $(\gamma_i, w_i) = \mathrm{RR}(H, S, Z)$, where $Z = [U_{i-1}\ u_{i;j}\ p_{i;j}]$
5 $\lambda_{i;j+1} = \gamma_i$, $u_{i;j+1} = Z w_i$

- ..., [Faddeev/Faddeeva'63],..., [Longsine/McCormick'80] for $K_{i;j} = I$, ...

PSD*id* assumptions

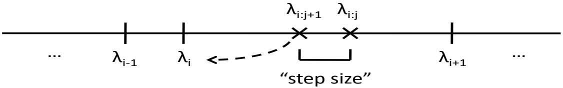
1. initialize $u_{i;0}$ such that $U_{i-1}^H S u_{i;0} = 0$ and $\|u_{i;0}\|_S = 1$
2. $\lambda_{i;0} = \rho(u_{i;0})$, Rayleigh quotient
3. the preconditioners $K_{i;j}$ are *effective positive definite*, namely,

$$K_{i;j}^{\mathrm{d}} \equiv (U_{i-1}^{\mathrm{c}})^T S K_{i;j} S U_{i-1}^{\mathrm{c}} > 0,$$

   where $U_{i-1}^{\mathrm{c}} = [u_i, u_{i+1}, \ldots, u_n]$.

PSD*id* properties

1. Z is of full column rank
2. $U_{i-1}^H S u_{i;j+1} = 0$ and $\|u_{i;j+1}\|_S = 1$
3. $\lambda_i \leq \lambda_{i;j+1} < \lambda_{i;j}$
4. $\lambda_{i;j} - \lambda_{i;j+1} \geq \sqrt{g^2 + \phi^2} - g =$ "step size" > 0,



5. $p_{i;j} = -K_{i;j} r_{i;j}$ is an *ideal search direction* if $p_{i;j}$ satisfies

$$U^T S(u_{i;j} + p_{i;j}) = (\times, \ldots, \times, \xi_i, 0, \ldots, 0)^T \quad \text{and} \quad \xi_i \neq 0. \qquad (3)$$

It implies that $\lambda_{i;j+1} = \lambda_i$.

PSD*id* convergence

If $\lambda_i < \lambda_{i;0} < \lambda_{i+1}$ and $\sup_j \mathrm{cond}(K^{\mathrm{d}}_{i;j}) = q < \infty$, then the sequence $\{\lambda_{i;j}\}_j$ is strictly decreasing and bounded from below by λ_i, i.e.,

$$\lambda_{i;0} > \lambda_{i;1} > \cdots > \lambda_{i;j} > \lambda_{i;j+1} > \cdots \geq \lambda_i$$

and as $j \to \infty$,

1. $\lambda_{i;j} \to \lambda_i$
2. $u_{i;j}$ converges to u_i *directionally*:

$$\|r_{i;j}\|_{S^{-1}} = \|Hu_{i;j} - \lambda_{i;j} S u_{i;j}\|_{S^{-1}} \to 0$$

PSD*id* convergence rate

Let $\epsilon_{i;j} = \lambda_{i;j} - \lambda_i$, then

$$\epsilon_{i;j+1} \leq \left[\frac{\mathit{\Delta} + \tau\sqrt{\theta_{i;j}\epsilon_{i;j}}}{1 - \tau(\sqrt{\theta_{i;j}\epsilon_{i;j}} + \delta_{i;j}\epsilon_{i;j})} \right]^2 \epsilon_{i;j}$$

provided that the i-th approximate eigenvalue $\lambda_{i;j}$ is **localized**, i.e.

$$\tau(\sqrt{\theta_{i;j}\epsilon_{i;j}} + \delta_{i;j}\epsilon_{i;j}) < 1,$$

where

- $\mathit{\Delta} = \frac{\mathit{\Gamma}-\gamma}{\mathit{\Gamma}+\gamma}$ and $\tau = \frac{2}{\mathit{\Gamma}+\gamma}$
- $\delta_{i;j} = \|S^{\frac{1}{2}} K_{i;j} S^{\frac{1}{2}}\|$ and $\theta_{i:j} = \|S^{\frac{1}{2}} K_{i;j} M K_{i;j} S^{\frac{1}{2}}\|$

$\mathit{\Gamma}$ and γ are largest and smallest pos. eigenvalues of $K_{i;j}M$ and $M = P_{i-1}^H (H - \lambda_i S) P_{i-1}$ and $P_{i-1} = I - U_{i-1} U_{i-1}^H S$

PSD*id* convergence rate, cont'd

Remarks:

1. If $K_{i;j} = I$, the convergence of SD proven in [Faddeev/Faddeeva'63,..., Longside/McCormick'80, ...]
2. If $i = 1$ and $K_{1;j} = K > 0$, it is Samokish's theorem (1958), which is first and still sharpest quantitative analysis [Ovtchinnikov'06].
3. Asymptotically,

$$\epsilon_{i;j+1} \leq \left[\mathit{\Delta} + \mathcal{O}(\epsilon_{i;j}^{1/2})\right]^2 \epsilon_{i;j}$$

4. Optimal $K_{i;j}$: $\mathit{\Delta} = 0 \rightsquigarrow$ quadratic conv.
5. Semi-optimal $K_{i;j}$: $\mathit{\Delta} + \tau\sqrt{\theta_{i;j}\epsilon_{i;j}} \to 0 \rightsquigarrow$ superlinear conv.
6. (Semi-)optimality depends on the eigenvalue distribution of $K_{i;j}M$

Locally accelerated preconditioner

Consider the preconditioner

$$\widehat{K}_{i;j} = \big(H - \beta_{i;j} S\big)^{-1} \quad \text{with} \quad \beta_{i;j} = \lambda_{i;j} - c\|r_{i;j}\|_{S^{-1}}$$

If

$$0 < \Delta_{i;j} < \min\{\frac{1}{4}\Delta_i^2, 0.1\} \quad \text{and} \quad c > 3\sqrt{\Delta_{i;j}}.$$

Then

1. $K_{i;j}$ is effective positive definite
2. $\lambda_{i;j}$ is localized
3. $\Delta + \tau\sqrt{\theta_{i;j}\epsilon_{i;j}} \to 0$

Therefore, $\widehat{K}_{i;j}$ is asymptotically optimal

PSD*id* $\rightsquigarrow$ LABPSD = Locally Accelerated BPSD

0 Initialize $U_{m+\ell;0} = [\, u_{1;0}\ u_{2;0}\ \ldots\ u_{m+\ell;0} \,]$
1 $(\Gamma, W) = \mathrm{RR}(H, S, U_{m+\ell;0})$
2 update $\Lambda_{m+\ell;0} = \Gamma$ and $U_{m+\ell;0} = U_{m+\ell;0} W$
3 for $j = 0, 1, \ldots,$ do
4 compute $R = HU_{m;j} - SU_{m;j}\Lambda_{m;j} \equiv [\, r_{1;j}\ r_{2;j}\ \ldots\ r_{m;j} \,]$
5 if $\mathrm{Res}[\Lambda_{m;j}, U_{m;j}] = \max_{1 \le i \le m} \mathrm{Res}[\lambda_{i;j}, u_{i;j}] \le \tau_{\mathrm{eig}}$, break
6 for $i = 1, 2, \ldots, m$
if $\lambda_{i;j}$ is **localized**, then solve $(H - \lambda_{i;j} S) p_{i;j} = -r_{i;j}$ for $p_{i;j}$
7 $(\Gamma_{m+\ell}, W_{m+\ell}) = \mathrm{RR}(H, S, Z)$, where $Z = [U_{m+\ell;j}\ P_j]$
8 update $\Lambda_{m+\ell;j+1} = \Gamma_{m+\ell}$ and $U_{m+\ell;j+1} = ZW_{m+\ell}$
9 end
10 return $\{(\lambda_{i;j}, u_{i;j})\}_{i=1}^{m}$

Note: A "global" preconditioner $\approx (H - \sigma S)^{-1}$ can be used to accelerate the "localization" and convergence of step 6.

Numerical example 1: Harmonic1D

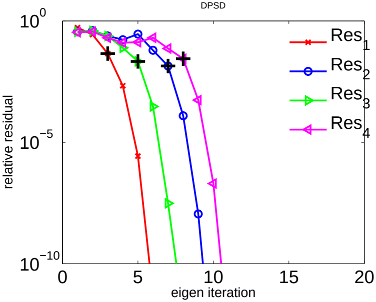
- PUFE discretization for harmonic oscillator in 1D
- $n = 112$ for 6-digit accuracy of 4 smallest eigenvalues $\lambda_1, \lambda_2, \lambda_3, \lambda_4$
- H and S are ill-conditioned

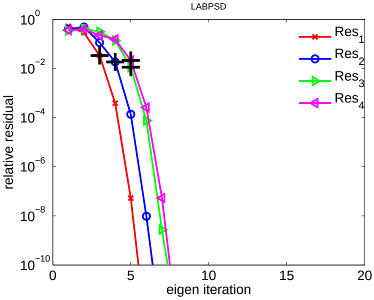
$$\text{cond}(H) = 8.79 \times 10^{10} \quad \text{and} \quad \text{cond}(S) = 2.00 \times 10^{12}$$

- H and S share a *near-nullspace* span$\{V\}$

$$\|HV\| = \|SV\| = O(10^{-5}) \quad \text{and} \quad \dim(V) = 17$$

- All computed $\widehat{\lambda}_1, \widehat{\lambda}_2, \widehat{\lambda}_3, \widehat{\lambda}_4$ have 6-digit accuracy.





Numerical example 2: CeAl-PUFE

- Metallic, triclinic CeAl, particularly challenging [Cai, B., Pask, Sukumar'13]
- $n = 5336$ from PUFE discretization of the Kohn-Sham equation
- H and S are ill-conditioned

$$\text{cond}(H) = 1.16 \times 10^{10} \quad \text{and} \quad \text{cond}(S) = 2.57 \times 10^{11}$$

- H and S share a *near-nullspace* span$\{V\}$

$$\|HV\| = \|SV\| = O(10^{-4}) \quad \text{and} \quad \dim(V) = 1000$$