Projection Methods for Generalized Eigenvalue Problems

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Outline

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The Generalized Eigenvalue Problem (GEP)

Definition

Let $K, M \in \mathbb{C}^{n,n}$. Finding $x \in \mathbb{C}^n \setminus \{0\}$ and $\lambda \in \mathbb{C}$ so that

$$Kx = \lambda Mx$$

is called a *generalized eigenvalue problem*.
K is called *stiffness matrix*, M is called *mass matrix*.
(λ, x) is called an *eigenpair*.

Matrix Properties

- K, M arise from finite element discretization
- K, M Hermitian positive semidefinite (HPSD)
- M may be diagonal

Solution Properties

Regular matrix pencils, HPSD matrices

- The matrices can be simultaneously diagonalized by a non-unitary congruence transformation
- $0 \leq \lambda \leq \infty$

Singular Matrix Pencils

Example

$$K = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, M = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}.$$

- $(K - \lambda M)e_2 = 0$ has a solution for all values of λ
- (K, M) is called *singular*

Outline

Requirements for Practical Accuracy Measures

- Can be calculated numerically stable
- Quickly computable
- Structure preserving
- Computes relative errors

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Polynomial Norms

Definition (Adhikari, Alam, and Kressner, 2011)

Let $K, M \in \mathbb{C}^{n,n}$, let $\omega \in \mathbb{R}^2$, $\omega > 0$, let $P(t) = K - tM$. We define the matrix polynomial norm $\|P\|_{\omega,p,q}$ as follows:

$$\|P\|_{\omega,p,q} := \|[1/\omega_1 \|K\|_p, 1/\omega_2 \|M\|_p]\|_q.$$

Structured Backward Error for Hermitian GEPs

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$$\Delta P(t) := \Delta K - t\Delta M.$$

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Definition

Let $(\widetilde{\lambda}, \widetilde{x})$ be an approximate eigenpair of the Hermitian matrix pencil (K, M). Then the *structured* backward error of $(\widetilde{\lambda}, \widetilde{x})$ is defined as

$$\eta^H_{\omega,p,q}(\widetilde{\lambda}, \widetilde{x}) := \min\{\|\Delta P\|_{\omega,p,q} : P(\widetilde{\lambda})\widetilde{x} + \Delta P(\widetilde{\lambda})\widetilde{x} = 0,\ \Delta P = \Delta P^*\}.$$

Structured Backward Error for Hermitian GEPs

Calculation

Theorem (Adhikari and Alam, 2011, Theorem 3.10)

Let $(\widetilde{\lambda}, \widetilde{x})$ be an approximate eigenpair of the Hermitian matrix pencil (K, M), where $\widetilde{\lambda}$ is real finite and $\|\widetilde{x}\|_2 = 1$. Let $r = K\widetilde{x} - \widetilde{\lambda} M \widetilde{x}$, let $\omega_{rel} = [\|K\|_F, \|M\|_F]$. Then

$$\eta^H_{\omega_{rel},F,2}(\widetilde{\lambda}, \widetilde{x}) = \min \left\| \left[\frac{\|\Delta K\|_F}{\|K\|_F}, \frac{\|\Delta M\|_F}{\|M\|_F} \right] \right\|_2 = \sqrt{\frac{2\|r\|_2^2 - |r^* \widetilde{x}|^2}{\|K\|_F^2 + |\widetilde{\lambda}|^2 \|M\|_F^2}},$$

where $(K + \Delta K)\widetilde{x} = \widetilde{\lambda}(M + \Delta M)\widetilde{x}$.

Outline

Solvers for GEPs with HPSD Matrices

Standard Eigenvalue Problem (SEP) Reduction (SR)

K Hermitian, M HPD:

- Compute Cholesky decomposition $LL^* := M$
- Solve $L^{-1}KL^{-*}x_L = \lambda x_L$
- Revert basis change: $x := L^{-T}x_L$

K Hermitian, M HPSD:

- Deflate infinite eigenvalues from matrix pencil
- Apply SEP reduction to deflated pencil

The Generalized Singular Value Decomposition (GSVD)

Definition (MC, §6.1.6, Bai, 1992, §2)

Let $n, r \in \mathbb{N}$, $n \geq r$, let $A, B \in \mathbb{C}^{n,r}$. Then there are unitary matrices $U_1, U_2 \in \mathbb{C}^{n,n}$, $Q \in \mathbb{C}^{r,r}$, nonnegative diagonal matrices $\Sigma_1, \Sigma_2 \in \mathbb{R}^{n,r}$, and an upper-triangular matrix $R \in \mathbb{C}^{r,r}$ such that

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 \\ \Sigma_2 \end{bmatrix} \begin{bmatrix} 0 & R \end{bmatrix} Q^*.$$

It holds that

$$\Sigma_1 = \begin{matrix} \\ r \\ n-r \end{matrix} \begin{matrix} r \\ \begin{bmatrix} C \\ 0 \end{bmatrix} \end{matrix}, \Sigma_2 = \begin{matrix} \\ r \\ n-r \end{matrix} \begin{matrix} r \\ \begin{bmatrix} S \\ 0 \end{bmatrix} \end{matrix},$$

where $C^2 + S^2 = I_r$. If A and B are real, then all matrices may be taken to be real.

Theorem (Bai, 1992, §4.2, §4.3)

Let $A, B \in \mathbb{C}^{n,n}$*, let* $\operatorname{rank}[A^*, B^*] = n$*, let*

$$\begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix} \begin{bmatrix} \Sigma_1 \\ \Sigma_2 \end{bmatrix} RQ^*$$

be the GSVD of (A, B) *and let* $QR^{-*} = [x_1, x_2, \dots, x_n]$*. Then we solved implicitly the generalized eigenvalue problem*

$$A^* A x_i = \lambda_i B^* B x_i,$$

where $\lambda_i = c_{ii}^2 / s_{ii}^2$*,* $i = 1, 2, \dots, n$*. If* A *and* B *are real, then all matrices can be taken to be real.*
Note (∞, x) *is an eigenpair of* $(A^* A, B^* B)$ *iff* $(0, x)$ *is an eigenpair of* $(B^* B, A^* A)$*.*

Solvers for GEPs with HPSD Matrices

GSVD Reduction

- Compute A such that $K = A^*A$
- Compute B such that $M = B^*B$
- Compute GSVD of (A, B)
    - Compute GSVD directly, or
    - use QR factorizations and a CS decomposition (QR+CSD)
- Compute eigenpairs

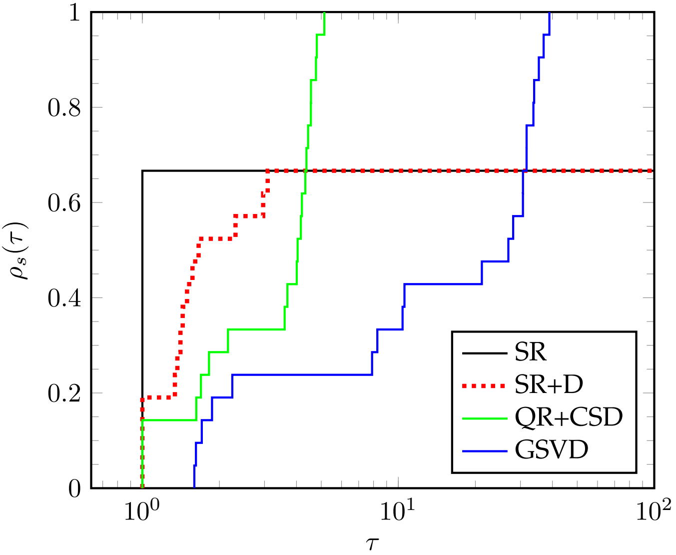
Solvers for GEPs with HPSD Matrices

Properties

Solver	QZ	SR	SR+D	GSVD
Backward stable	✓		(✓)	✓
Computes eigenvectors		✓	✓	✓
Preserves symmetry		✓	✓	✓
Preserves definiteness		(✓)	(✓)	✓
Handles singular pencils	✓		(✓)	✓
(K, M), (M, K) equivalent	✓			✓

Solvers for GEPs with HPSD Matrices

Performance Profile (Single Precision)



Outline

Projection Method

Definition (Saad, 2011, §4.3)

Given a subspace $\mathcal{S} \subseteq \mathbb{C}^n$, an orthogonal *projection method* for an eigenvalue problem tries to approximate an eigenpair $(\widetilde{\lambda}, \widetilde{x})$ so that $\widetilde{x} \in \mathcal{S}$ and $K\widetilde{x} - \widetilde{\lambda}M\widetilde{x} \perp \mathcal{S}$ for some given inner product in which orthogonality is defined.

A Multilevel Eigensolver

Assumptions

- The user seeks eigenpairs (in contrast to eigenvalues),
- mass and stiffness matrix are given explicitly,
- mass and stiffness matrix are HPSD,
- the matrix pencil is regular, and
- GEPs on the block diagonal deliver good approximations to the eigenpairs.

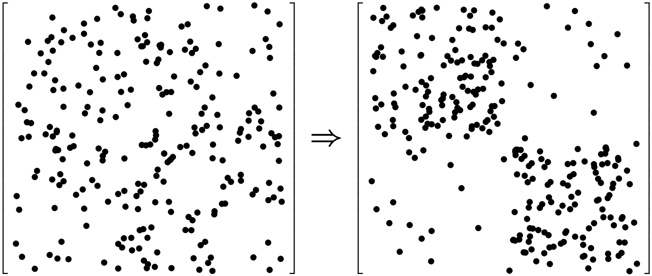
A Multilevel Eigensolver

Idea

Recursively decompose the GEP into many small GEPs

A Multilevel Eigensolver

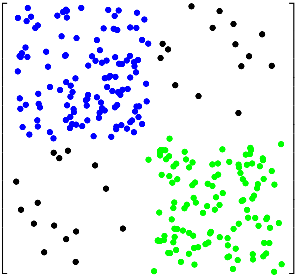
Step 1: Partitioning

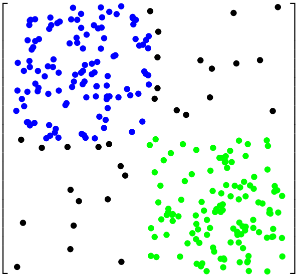


Minimize weight of off-diagonal entries (graph bisection)

A Multilevel Eigensolver

Step 2: Recursion

$K =$ 

$M =$ 

Compute eigenpair approximations in block diagonal GEPs

A Multilevel Eigensolver

Step 3: Iterative Improvement

$K =$ 

$M =$ 

Improve eigenpair approximations

Outline

Additional Thesis Topics

- Singular matrix pencils
- A new fast and stable GEP solver for HPSD matrices
- Improving numerical stability
- Numerical experiments with multilevel eigensolver (TODO)

Conclusion

- Structured backward errors can be computed quickly for GEPs with Hermitian matrices
- GSVD-based solvers are fast and robust in practice
- In our tests the more robust the GEP solver, the slower the GEP solver

Thank you for your attention.
Questions?

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