Symmetric Indefinite Generalized Eigenproblems

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Symmetric Indefinite GEP

$$Ax = \lambda Bx, \quad A = A^T, \; B = B^T.$$

- A, B are indefinite.
- Eigenvalues can be complex.
- Set of left and right eig'vectors coincide.

Indefinite GEPs occur when solving symmetric QEPs

$$(\lambda^2 M + \lambda D + K)x = 0.$$

Open problem : derive method of solution that

- takes advantage of the symmetry,
- is efficient and numerically robust.

Some Methods

Assume that

- $A - \lambda B$ is regular and B nonsingular.
- (A, B) reduced to tridiagonal-diagonal form (T, J). [F.T. 2003]

Eigenvalues can be computed with

- Ehrlich-Aberth iteration
- HR algorithm
- LR algorithm
- Uhlig's DQR algorithm

Ehrlich-Aberth Method

Approximate simultaneously all the zeros of $p(z)$.
Given $z^{(0)} \in \mathbb{C}^n$, generates a sequence $z^{(j)} \in \mathbb{C}^n$

$$z_j^{(k+1)} = z_j^{(k)} - \frac{\frac{p(z_j^{(k)})}{p'(z_j^{(k)})}}{1 - \frac{p(z_j^{(k)})}{p'(z_j^{(k)})} \sum_{k=1,k\neq j}^{n} \frac{1}{z_j^{(k)} - z_k^{(k)}}}, \quad j = 1\colon n,$$

which locally converges to the n roots of $p(z)$.

Issues to be considered:

- Fast and stable computation of the Newton correction $p(z)/p'(z)$.
- Criterion for choosing initial approximations $z^{(0)}$.

Newton Correction $p(\lambda)/p'(\lambda)$

$p(\lambda) = \det(T - \lambda I)$, $T = \mathrm{tridiag}(\beta, \alpha, \gamma)$.

- **Three term recurrence:**
  compute $p(\lambda) = p_n(\lambda)$ and its derivative via

$$\begin{aligned} &p_0(\lambda) = 1, \quad p_1(\lambda) = \alpha_1, \\ &p_k(\lambda) = (\alpha_k - \lambda) p_{k-1}(\lambda) - \beta_{k-1}\gamma_{k-1} p_{k-2}(\lambda), \qquad k = 2\colon n. \end{aligned}$$

  Suffers from overflow/underflow problems.

- **Trace representation:**

$$\frac{p'(\lambda)}{p(\lambda)} = -\sum_{j=1}^{n} \frac{1}{\lambda_j - \lambda} = -\,\mathrm{trace}(T - \lambda I)^{-1}.$$

Trace$(T - \lambda I)^{-1}$ in $O(n)$ ops

Let $S = QR$ be QR fact. of $S = T - \lambda I$ obtained using $n-1$ Givens rotations:

$$G_j([j, j+1], [j, j+1]) = \begin{bmatrix} \phi_j & \psi_j \\ -\overline{\psi}_j & \overline{\phi}_j \end{bmatrix}, \quad |\phi_j|^2 + |\psi_j|^2 = 1.$$

R is upper triangular with three superdiagonals r, s, t:

$$\begin{array}{lll} \tau_j = 1/\sqrt{|\widetilde{\alpha}_j|^2 + \beta_j^2}, & \phi_j = \overline{\widetilde{\alpha}}_j \tau_j, & \psi_j = \beta_j \tau_j, \\ r_j = \phi_j \widetilde{\alpha}_j + \psi_j \beta_j, & s_j = \phi_j \widetilde{\gamma}_j + \psi_j \alpha_{j+1}, & t_j = \psi_j \gamma_{j+1}, \\ \widetilde{\alpha}_{j+1} = -\psi_j \widetilde{\gamma}_j + \overline{\phi}_j \alpha_{j+1}, & \widetilde{\gamma}_{j+1} = \overline{\phi}_j \gamma_{j+1}, & \end{array}$$

for $j = 1 \colon n-1$, with $\widetilde{\alpha}_1 = \alpha_1$ and $\widetilde{\gamma}_1 = \gamma_1$.

Structure of Q

Semiseparable struct. of Q crucial to get $(S^{-1})_{jj}$ in $O(n)$ ops.

$$G_j([j,j+1],[j,j+1]) = \begin{bmatrix} \phi_j & \psi_j \\ -\overline{\psi_j} & \overline{\phi_j} \end{bmatrix}, \quad |\phi_j|^2 + |\psi_j|^2 = 1.$$

$$Q^* = G_{n-1} \cdots G_2 G_1 = \begin{bmatrix} v_1 u_1 & \psi_1 & & & 0 \\ v_2 u_1 & v_2 u_2 & \psi_2 & & \\ \vdots & \vdots & \ddots & \ddots & \\ \vdots & & & v_{n-1} u_{n-1} & \psi_{n-1} \\ v_n u_1 & v_n u_2 & \cdots & v_n u_{n-1} & v_n u_n \end{bmatrix},$$

where

$$u = D^{-1}[1, \overline{\phi_1}, \overline{\phi_2}, \ldots, \overline{\phi_{n-1}}]^T, \; v = D[\phi_1, \phi_2, \phi_3, \ldots, \phi_{n-1}, 1]^T,$$
$$D = \operatorname{diag}(1, -\psi_1, \psi_1\psi_2, \ldots, (-1)^{n-1}\psi_1\psi_2\cdots\psi_{n-1}).$$

Computing $\mathrm{trace}((T-\lambda I)^{-1})$

Let $T-\lambda I = QR$, w solution to $Rw = v$,
$D = \mathrm{diag}(1, -\psi_1, \psi_1\psi_2, \ldots, (-1)^{n-1}\psi_1\psi_2\cdots\psi_{n-1})$,
$u = D^{-1}[1, \bar{\phi}_1, \bar{\phi}_2, \ldots, \bar{\phi}_{n-1}]^T$,
$v = D[\phi_1, \phi_2, \phi_3, \ldots, \phi_{n-1}, 1]^T$.

Using structure of Q^* gives

$$(T-\lambda I)^{-1}_{jj} = e_j^* R^{-1} Q^* e_j = u_j w_j \quad \Leftrightarrow \quad \mathrm{trace}((T-\lambda I)^{-1}) = u^T w.$$

Stable process if diagonal scaling of R is used to solve $Rw = v$.

Requires $O(n)$ ops.

Initial Approximations

Use a divide and conquer strategy :

$$T = \begin{bmatrix} T_1 & 0 \\ 0 & T_2 \end{bmatrix} + uv^T.$$

Approximate eig'vals of T by eig'vals of $T_1 \oplus T_2$.

- Unlike symmetric case, no obvious connection between eigenvalues of $T_1 \oplus T_2$ and T.
- Have heuristic arguments to support this strategy.
- Works well in practice.

Numerical Experiments

`aberth`: implementation of Ehrlich-Aberth iterations.
`dhseqr`: LAPACK implementation of QR alg.

Conducted numerous tests on tridiagonal matrices with various spectrum and eigenvalue condition numbers.

Summary:

- Eigenvalues computed by `aberth` tend to be more accurate, in particular for eigenvalues with small moduli.
- `aberth` less affected than `dhseqr` by large eigenvalue condition numbers.
- `aberth` faster than `dhseqr` for large n.

Example 1

T has three clusters of eigenvalues, $n = 20$.

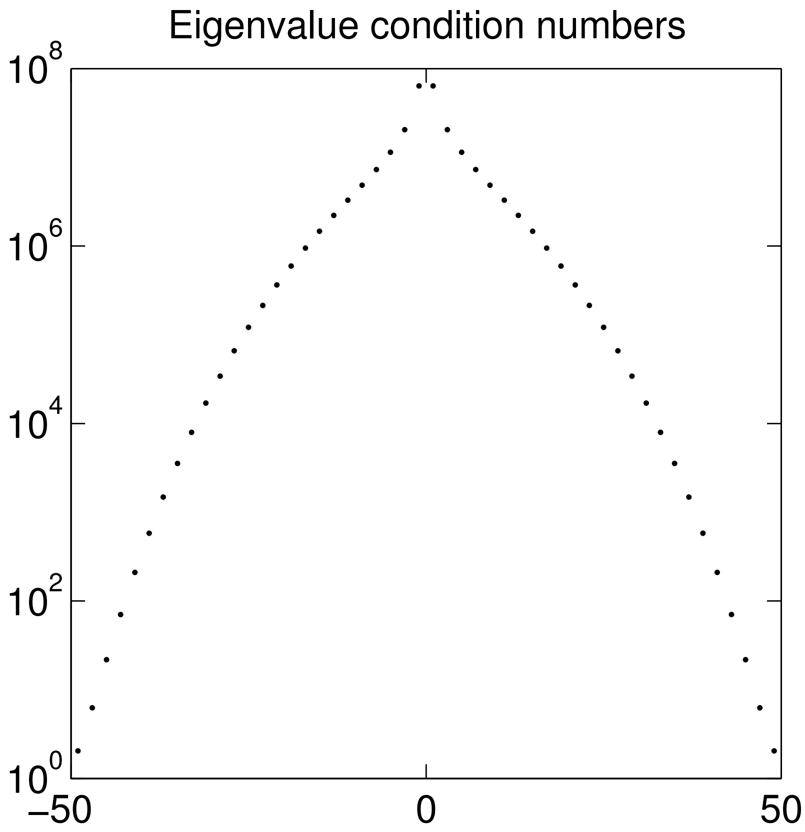
$$\kappa(\lambda) = \frac{\|x\|_2 \|y\|_2 \|T\|_2}{|\lambda| \, |y^T x|}$$

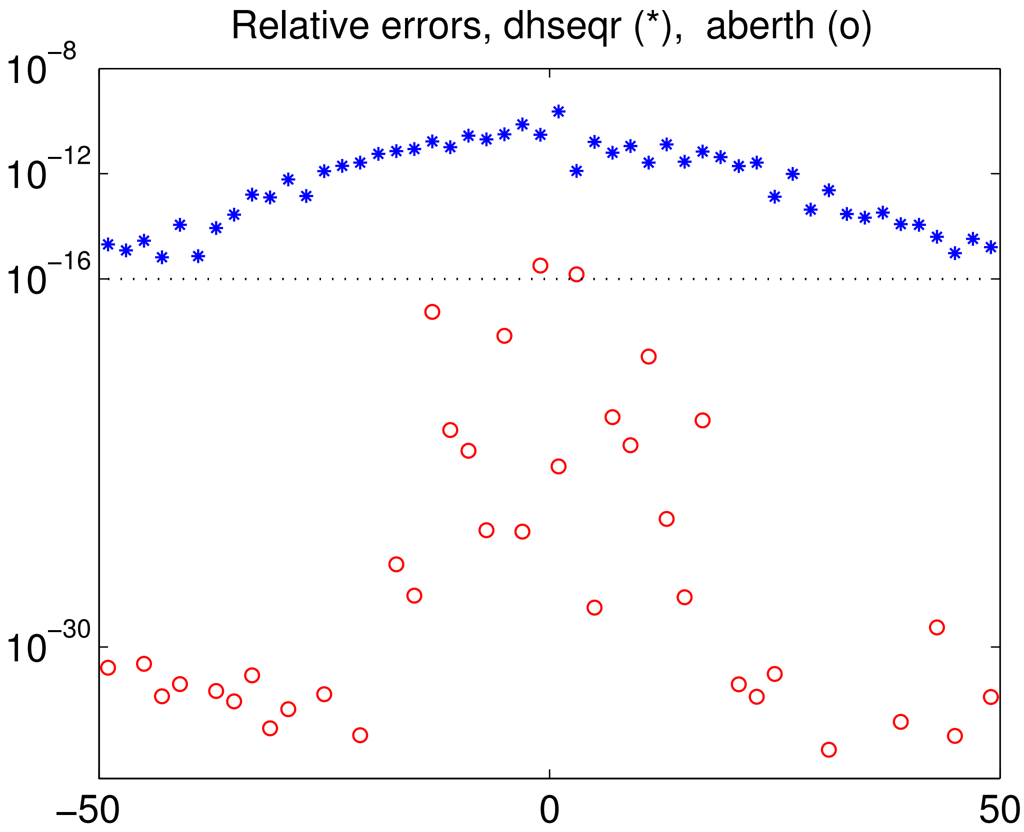
		$\max_i \; |\lambda_i - \hat{\lambda}_i| / |\lambda_i|$	
	$\kappa(\lambda)$	`dhseqr`	`aberth`
$\lambda \approx -10^5$	1.2	3e-16	8e-18
$\lambda \approx 10^5$	2e2	1e-13	1e-14
$|\lambda| \approx 10^{-5}$	1e10	4e-7	1e-16

Clement Matrix

$$T = \mathrm{tridiag}(\beta, 0, \gamma), \;\; \beta_j = \gamma_{n-j}, \;\; \gamma_j = j, \, j = 1\colon n-1.$$

$$n = 50\colon \Lambda(T) = \{-49, -47, \ldots, -1, 1, \ldots, 47, 49\}.$$





Part 2: HZ Algorithm

$$Tx = \lambda Jx, \qquad J \in \operatorname{diag}_p^n(\pm 1).$$

Variant of Bunse-Gerstner HR iteration [1981].

kth HZ step:

$$\begin{aligned} p_k(J_{k-1}T_{k-1}) &= H_k R_k, \quad \text{(HR factorization)} \\ J_k &= H_k^T J_{k-1} H_k, \\ T_k &= H_k^T T_{k-1} H_k. \end{aligned}$$

- H_k is (J_{k-1}, J_k)-orthogonal.
- Iteration preserves symm. and tridiagonal form.
- T_k converges to block-diagonal form with 1×1 and 2×2 blocks.

HR Factorization

$A = HR$ is an HR factorization of $A \in \mathbb{R}^{n \times n}$ w.r.t. $J \in \mathrm{diag}_p^n(\pm 1)$ if R is upper triangular and $H^T J H = \widetilde{J}$.

Theorem 1 (Bunse-Gerstner, 81)
$A \in \mathbb{R}^{n \times n}$ has an HR factorization with respect to $J \in \mathrm{diag}_p^n(\pm 1)$ iff all principal minors of $A^T J A$ are nonzero.

Consider HZ algorithm with double shift strategy:

$$p(x) = (x - \sigma)(x - \rho), \quad \sigma = \bar{\rho} \text{ if } \sigma \in \mathbb{C}.$$

Theorem 2 *If σ is a defective ei'val of $T - \lambda J$ then $p(JT)$ does not have an HR factorization.*

For single shift, Wiberg [97] showed $JT - \sigma I = HR$ fails to exist when σ is any complex ei'val.

Practical Implementation

HZ step: $$p(JT) = HR,$$ implemented implicitly

$$\widehat{T} = H^T T H, \quad \widehat{J} = H^T J H.$$

$$T_0 = H_0^T T H_0 = \begin{bmatrix} \times & \times & \times & \times & & \\ \times & \times & \times & \times & & \\ \times & \times & \times & \times & & \\ \times & \times & \times & \times & \times & \\ & & & \times & \times & \times \\ & & & & \times & \times \end{bmatrix}.$$

- Bulge chased with Givens and hyperbolic rotations.
- Strategy: minimize number of hyperbolic rot. used.
- Apply hyperbolic rotations G in a mixed way ($G = LU$).
- Monitor conditioning of transformations.

Bulge Chasing Strategy

Hyperbolic rotation: $G = \begin{bmatrix} c & s \\ s & c \end{bmatrix}$, $c^2 - s^2 = \pm 1$

satisfies $G^T J G = \pm J$, $J = \left[\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right]$. If $x^T J x \neq 0$,

$$(c, s) = (x_1, -x_2)/\sqrt{|x^T J x|} \quad \Rightarrow \quad \boxed{Gx = \rho e_1}.$$

Consider 4×4 matrix pair:

$$T = \begin{bmatrix} \times & x_1 & x_2 & x_3 \\ x_1 & \times & \times & \times \\ x_2 & \times & \times & \times \\ x_3 & \times & \times & \times \end{bmatrix}, \quad J = \begin{bmatrix} 1 & & & \\ & -1 & & \\ & & -1 & \\ & & & 1 \end{bmatrix}, \quad |x_1| < |x_2| < |x_3|.$$

- To zero x_3 first and then x_2 one needs two hyperb. rots.
- Zero x_2 with Givens and x_3 with hyperbolic rotation.

Numerical Comparison

`dhseqr`: LAPACK implementation of QR alg.

`aberth` : Ehrlich-Aberth iterations.

`thz`: double-shift HZ algorithm.

`tlr`: double-shift LR algorithm.

$$\kappa(\lambda) = \frac{\|x\|_2 \|y\|_2 \|T\|_2}{|\lambda| \, |y^T x|}$$

Test matrices, $n = 20$		1	4	5	7
$\max_i \kappa(\lambda_i)$		1e3	2.4	1e10	3e2
$\max_i \frac{\lvert\lambda_i - \hat{\lambda}_i\rvert}{\lvert\lambda_i\rvert}$	`dhseqr`	8e-15	5e-15	1e-6	6e-15
	`aberth`	1e-16	2e-16	3e-14	3e-16
	`thz`	3e-13	5e-13	2e-6	2e-13
	`tlr`	9e-15	3e-11	fail	1e-11

Eigenvalue Error Bounds

Objective : cheap computable error bounds for ei'vals of tridiagonal matrices.

$\mathcal{D}(a,\rho)$: disk of center a and radius ρ.

Lemma 1 (Carstensen 91) *Assume $p(\lambda)$ is monic, of degree n and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be distinct. Let*

$$\rho_\ell = \frac{n|p(\lambda_\ell)|}{\left|\prod_{\substack{j=1\\ j\neq \ell}}^{n} (\lambda_\ell - \lambda_j)\right|}.$$

Then $\mathcal{U} = \bigcup_\ell \mathcal{D}(\lambda_\ell, \rho_\ell)$ contains all the zeros of $p(\lambda)$. In particular, any isolated disk contains a single zero.

Rounding errors $\Rightarrow fl(\rho_\ell) = \widehat{\rho}_\ell$ may be inaccurate $\Rightarrow$ $\mathcal{D}(\lambda_\ell, \widehat{\rho}_\ell)$ may not provide a set of inclusion disks.

Eigenvalue Error Bounds Cont.

$\widehat{\ }$ denotes computed quantities, u: unit roundoff.

Assume we know an upper bound Δp_ℓ for $\big||\hat{p}_\ell| - |p(\lambda_\ell)|\big|$. Let

$$\widetilde{\rho}_\ell = (1+2nu)n(|\hat{p}_\ell| + \Delta p_\ell) \Big/ fl\Big(\big|\prod_{\substack{j=1\\ j\neq \ell}}^{n}(\lambda_\ell - \lambda_j)\big|\Big).$$

The set $\{\mathcal{D}(\lambda_\ell, \widetilde{\rho}_\ell),\ \ell = 1\colon n\}$ is a set of inclusion disks.

How to determine Δp_ℓ?

Computing Δp_ℓ

Let $T - \lambda_\ell I = QR$. Then $|p(\lambda_\ell)| = \prod_{j=1}^{n} |r_{jj}|$.
Write

$$\widehat{r}_{jj} = r_{jj} + \delta r_{jj}, \qquad |\delta r_{jj}| \leq \Delta r_{jj}.$$

Then

$$\Delta p_\ell = |\widehat{p}_\ell| \left(\sum_{j=1}^{n} \Delta r_{jj} / |\widehat{r}_{jj}| + (n-1) 2\sqrt{2} u \right).$$

Δr_{jj} are computed along with $\widehat{r}_{jj} = fl(r_{jj})$ thank to a systematic running error analysis.

- Computing the upper bound $\widetilde{\rho}_\ell$ is inexpensive: $O(n)$ ops per ei'val.
- $\widetilde{\rho}_\ell$ comes for free if one use Ehrlich-Aberth.

Example 2

$$T = D^{-1}\,\mathrm{tridiag}(1,\alpha,1),\;\; \alpha_j = 10^{6(-1)^{j+1}},\; \begin{cases} \delta_j=1, j\le n/2, \\ \delta_j=-1, j>n/2 \end{cases}.$$

$\widetilde{\rho}(\lambda)$: rel. error bound on λ
$\kappa_s(\lambda)$: ei'val. struct. cond. number
$\eta_s(\lambda)$: ei'val. struct. backward err.

$$\frac{|\lambda-\hat{\lambda}|}{|\lambda|} \le \begin{cases} \widetilde{\rho}(\lambda) \\ \kappa_s(\lambda)\times\eta_s(\lambda). \end{cases}$$

λ	$\lvert\lambda-\hat{\lambda}\rvert/\lvert\lambda\rvert$	$\widetilde{\rho}(\lambda)$	$\kappa_s(\lambda)$	$\eta_s(\lambda)$
$-$1.0e+6	0	2e-24	0.7	2e-22
$-$1.7e-6	7e-9	7e-8	5e11	2e-20
$-$7.4e-7	1e-4	1e-3	1e12	2e-16
2.2e-7 $\pm$ i5.0e-7	4e-6	4e-5	1e12	5e-18
1.0e+6	0	8e-17	0.7	2e-16

- $\kappa_s(\lambda)$ and $\eta_s(\lambda)$ require ei'vect. Expensive to compute.
- Only $O(n)$ ops. to compute $\widetilde{\rho}(\lambda)$.

Towards a Robust Algorithm

1. Reduce $A - \lambda B$ to tridiag.-diag. form $T - \lambda J$ ($O(n^3)$ ops.)
2. Compute eigenvalues with HZ algorithm ($O(n^2)$ ops.)
3. Refine eigenvalues with modified Ehrlich-Aberth iter. ($O(n)$ ops. per ei'val.)
4. Compute eigenvectors of (T, J) with differential-qd alg. ($O(n)$ ops. per ei'vec.)
5. Recover eigenvectors of (A, B) ($O(n^2)$ ops. per ei'vec.)
6. Compute structured backward error of (x, λ) ($O(n^2)$ ops. per eigenpair)
7. If necessary, refine (x, λ) ($O(n^2)$ ops. per eigenpair)

Papers and Reports

- [F.T] Tridiagonal-Diagonal Reduction of Symmetric Indefinite Pairs, NA Report 409, 2002. To appear in SIMAX.
- [D. Bini, L. Gemignani, F.T.] The Ehrlich-Aberth Method for the Nonsymmetric Tridiagonal Eigenvalue Problem, NA Report 428, 2003, revised 2004.
- [M. Berhanu, F.T.] A Robust Implementation of the HZ Algorithm, NA Report in preparation.

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