Recent Developments in Symmetric Quadratic Eigenvalue Problems

Françoise Tisseur
Department of Mathematics
University of Manchester

ftisseur@ma.man.ac.uk
http://www.ma.man.ac.uk/~ftisseur/

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Quadratic Eigenvalue Problems

$n \times n$ quadratic matrix polynomial

$$Q(\lambda) = \lambda^2 M + \lambda C + K.$$

Find scalars λ and nonzero vectors x, y s.t.

$$Q(\lambda)x = 0, \quad y^* Q(\lambda) = 0, \quad x, y \neq 0.$$

A nonsingular implies Q has $2n$ £nite eigenvalues: the roots of $\det(Q(\lambda)) = 0$.

When A is singular, the degree of $\det(Q(\lambda)) = r < 2n$ and Q has r £nite eigenvalues and $2n - r$ in£nite eigenvalues.

Example

$$M = \begin{bmatrix} 0 & 6 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & -6 & 0 \\ 2 & -7 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad K = I.$$

$Q(\lambda) = \lambda^2 M + \lambda C + K$ is regular: $\det Q(\lambda) \not\equiv 0$.

Six eigenpairs (λ_k, x_k), $k = 1\colon 6$, given by

k	1	2	3	4	5	6
λ_k	$1/3$	$1/2$	1	i	$-i$	∞
x_k	$\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$	$\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$

Classes of QEPs

Matrix	Eigenvalue	Eigenvector
M nonsingular	$2n$ £nite λ's	
M singular	£nite , ∞ λ's	
M, C, K real	λ's real or come in pairs $(\lambda, \bar{\lambda})$	x right ei'vec of λ, right ei'vec of $\bar{\lambda}$
M, C, K Hermitian	λ's real or come in pairs $(\lambda, \bar{\lambda})$	x right ei'vec of λ , x le ei'vec of $\bar{\lambda}$
$M > 0$, $C, K \geq 0$	$\Re(\lambda) \leq 0$	
$M, C > 0$, $K \geq 0$, $\gamma(M, C, K) > 0$	λ's real, gap between n larg./small. λ.	n lin. ind. ei'vecs co to n largest λ's.
M, K Hermitian, $M > 0$, $C = -C^*$	λ's purely imaginary or come in pairs $(\lambda, -\bar{\lambda})$	x right ei'vec of λ, x le ei'vec of $-\bar{\lambda}$
$M, K > 0$ real, $C = -C^T$	λ's purely imaginary	

$$\gamma(M, C, K) = \min_{||x||_2=1} \left[(x^* C x)^2 - 4(x^* M x)(x^* K x) \right]$$

Outline

- Applications
- Hyperbolic and elliptic QEPs
  - Testing for hyperbolicity
  - Distance to non hyperbolic/elliptic QEP
- Numerical methods for symmetric QEPs
  - Reduction to simple forms
  - Eigensolvers for tridiagonal-diagonal symm. pairs
  - Structure preserving algorithms

Vibration Analysis of Structural Systems

Undamped structural eigenproblem in engineering

$$\lambda^2 Mx + Kx = 0.$$

In practice systems are subject to damping

$$\lambda^2 Mx + \lambda Cx + Kx = 0.$$

Proportional or Rayleigh damping: $C = \alpha M + \beta K$.
Damped QEP transformed to n decoupled eq.

Modern structures lead to non-classically damped eigenproblems

$$\lambda^2 Mx + \lambda Cx + Kx = 0.$$

Some More Applications

- Constrained least squares problem

$$\min_{x^T x = \alpha^2} \left\{ x^T A x - 2 b^T x \right\},$$

  where $A = A^T \in \mathbb{R}^{n \times n}, \; b \in \mathbb{R}^n$.

  The solution is $x = (A - \lambda I)^{-1} b$, where λ is the smallest eigenvalue of

$$\left(\lambda^2 I - 2\lambda A + (A^2 - \alpha^{-2} b b^T) \right) y = 0.$$

- Signal Processing (Davila's subspace approach).

Hyperbolic and Overdamped Systems

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

The QEP is Hermitian if M, C, K are Hermitian.

De£nition 1 *The QEP is hyperbolic if it is Hermitian with* $M > 0$ *and* $(x^*Cx)^2 > 4(x^*Mx)(x^*Kx)$ *for all* $x \neq 0$.

For any eigenpair (x, λ), $\lambda^2 x^*Mx + \lambda x^*Cx + x^*Kx = 0$, with solutions

$$\lambda = \left(-x^*Cx \pm \sqrt{(x^*Cx)^2 - 4(x^*Mx)(x^*Kx)}\right) / (2x^*Mx) \; .$$

De£nition 2 *The QEP is overdamped if it is hyperbolic with* $C > 0$ *and* $K \geq 0$.

For overdamped problems, $\lambda_i \leq 0$.

Elliptic Systems

De£nition 3 *The QEP is elliptic if it is Hermitian with $M > 0$ and*

$$(x^*Cx)^2 < 4(x^*Mx)(x^*Kx) \quad \textit{for all } x \neq 0.$$

Elliptic QEPs have nonreal eigenvalues, and, necessarily, K is pos. def.

Theorem 1 *Ellipticity of an Hermitian QEP with $M > 0$ is equivalent to either of the conditions*

1. *$Q(\mu) > 0$ for all $\mu \in \mathbb{R}$,*
2. *$(x^*Cx)^2 < 4(x^*Mx)(x^*Kx)$ for all ei'vectors x of the QEP.*

Testing for Hyperbolicity

Theorem 2 *Hermitian QEP with $M > 0$ is hyperbolic iff $Q(\mu) < 0$ for some $\mu \in \mathbb{R}$.*

Theorem 3 *The Hermitian QEP with $M > 0$ is hyperbolic iff the pair (A, B) is de£nite, where*

$$A = \begin{bmatrix} -K & 0 \\ 0 & M \end{bmatrix}, \quad B = -\begin{bmatrix} C & M \\ M & 0 \end{bmatrix}.$$

Proof. (A, B) de£nite iff $\alpha A + \beta B > 0$ for some α, β. Assume $\alpha \neq 0$,

$$\alpha A + \beta B = \begin{bmatrix} I & -\frac{\beta}{\alpha} I \\ 0 & I \end{bmatrix} \begin{bmatrix} -\alpha K - \beta C - \frac{\beta^2}{\alpha} M & 0 \\ 0 & \alpha M \end{bmatrix} \begin{bmatrix} I & 0 \\ -\frac{\beta}{\alpha} I & I \end{bmatrix}.$$

So $\alpha A + \beta B$ is congruent to $\alpha \operatorname{diag}(-(\mu^2 M + \mu C + K), M)$, where $\mu = \beta/\alpha$. The result follows from Theorem 2, since $M > 0$. $\square$

Distance to non-Hyperbolic/Elliptic QEP

Let $W(x, M, C, K) = \begin{bmatrix} 2x^*Mx & x^*Cx \\ x^*Cx & 2x^*Kx \end{bmatrix}$.

Note that $\det(W) \begin{cases} < 0 \;\; \forall\, x \neq 0 \text{ if QEP hyperbolic,} \\ > 0 \;\; \forall\, x \neq 0 \text{ if QEP elliptic.} \end{cases}$

$$d(M, C, K) = \min \{\, f(\Delta M, \Delta C, \Delta K) : \\ \det(W(x, M + \Delta M, C + \Delta C, K + \Delta K)) = 0 \text{ for some } x \neq 0 \,\}.$$

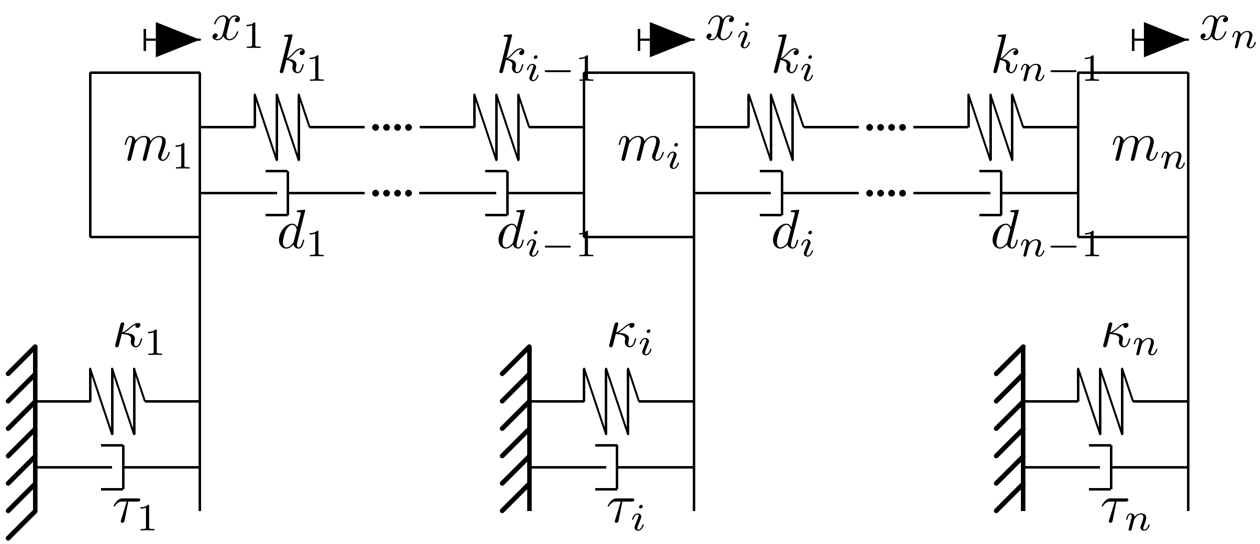
We have

$$d(M, C, K) = \min_{\|x\|_2 = 1} g(x),$$

where $g(x) = |\lambda_{\mathrm{opt}}(W(x, M, C, K))|$ and λ_{opt} ei'values smallest modulus.

For hyperbolic problems, $g(x)$ is differentiable for all nonzero x.

Mass-Spring System



QEP is overdamped.

- Bisection alg applied to (A, B) diagnoses pair de£nite, hence QEP hyperbolic, after 1 iteration.
- Computing $d(M, C, K)$ via unconstrained minimization of $\min_x g(x/\|x\|_2)$ shows $d(M, C, K) = 2.0$, with optimal perturbations

$$\Delta A = 0.125ee^T, \ \Delta B = -0.25ee^T, \ \Delta C = 0.125ee^T.$$

Wave Equation

$$\begin{cases} u_{tt} + \epsilon a(x) u_t = \Delta u, \quad x \in [0, \pi], \quad \epsilon > 0, \\ u(t, 0) = u(t, \pi) = 0. \end{cases}$$

Approximating $u(x,t) = \sum_{k=1}^{n} q_k(t) \sin(k\pi x)$ and applying Galerkin method leads to

$$M\ddot{q}(t) + C\dot{q}(t) + Kq(t) = 0,$$

where $q(t) = [\, q_1(t), \ldots, q_n(t)\,]^T$, $M = (\pi/2)I_n$, $K = (\pi/2)\mathrm{diag}(j^2)$, and

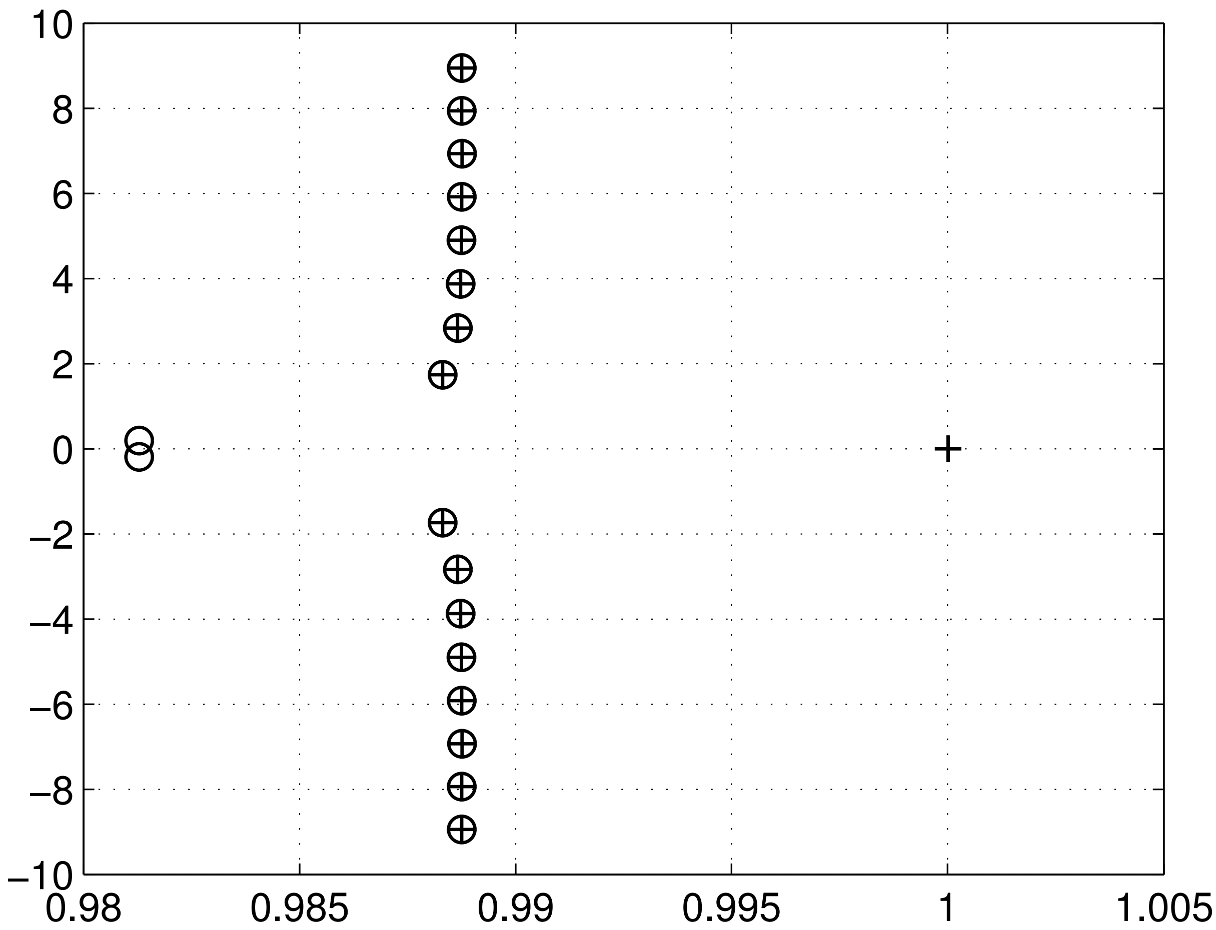
$$C = (c_{kj}), \quad c_{kj} = \int_0^{\pi} \epsilon\, a(x) \sin(kx) \sin(jx)\, dx.$$

We took $n = 9$, $a(x) = x^2(\pi - x)^2 - \delta$, $\delta = 201$, $\epsilon = 0.1$.

The QEP is elliptic.
We found $d(M, C, K) = 0.06$.

Spectrum for Wave Equation

Ei'vals of original elliptic QEP marked "$\circ$" and those of perturbed QEP "$+$"



Second Order Systems

Undamped multi-degree of freedom second-order systems

$$M\ddot{q} + C\dot{q} + Kq = Pf, \quad r = P^T q$$

leads to £rst order systems

$$Ap + B\dot{p} = Gf, \quad s = G^T p, \qquad p = [q^T, \dot{q}^T]^T.$$

Three types of analysis

- Computation of transient response $p(t)$,
  $\ddot{p}(t) = B^{-1}(Gf(t) - Ap(t))$.
- Computation of steady-state frequency response
  $r(\omega) = G^T(A - \omega^2 B)^{-1} Gf(\omega)$.
- Computation of natural frequencies ω_n (determined from ei'vals.).

Linearizing Symmetric QEPS

$$Q(\lambda) = \lambda^2 M + \lambda C + K.$$

First companion form:

$$A - \lambda B = \begin{bmatrix} 0 & W \\ -K & -C \end{bmatrix} - \lambda \begin{bmatrix} W & 0 \\ 0 & M \end{bmatrix}.$$

Second companion form:

$$A - \lambda B = \begin{bmatrix} -K & 0 \\ 0 & W \end{bmatrix} - \lambda \begin{bmatrix} C & M \\ W & 0 \end{bmatrix},$$

W can be any nonsingular $n \times n$ matrix.

Taking $W = -K$ in the £rst companion form $W = M$ in the second companion form yield two symmetric linearizations.

Reduction to Simple Forms

A, B: $n \times n$ symmetric (inde£nite) matrices.

Aim: Find W nonsingular such that $W^T AW$ and $W^T BW$ are in reduced form (tridiagonal, diagonal . . .).

Two reductions requiring a £nite number of steps:

- Simultaneous tridiagonalization of (A, B).
  Useful for transient response and steady state computation.
- Reduction to tridiagonal-diagonal form.
  First step in most eigensystem computation.
  Most compact form.

Simultaneous Tridiagonalization

S.D. Garvey, F.T., M. Friswell, J. Penny and U. Prells [2002]

No hyp. made on nonsingularity or de£niteness of A, B.

Basic idea: Assume there exists G_1 nonsingular such that

$$A_1 = G_1^T A G_1 = \begin{bmatrix} \kappa_1 & \tau_1 e_1^T \\ \tau_1 e_1 & \widetilde{A}_1 \end{bmatrix}, \; B_1 = G_1^T B G_1 = \begin{bmatrix} \mu_1 & \sigma_1 e_1^T \\ \sigma_1 e_1 & \widetilde{B}_1 \end{bmatrix},$$

$e_1 = [1, 0, \ldots, 0]^T$, $\kappa_1, \tau_1, \mu_1, \sigma_1 \in \mathbb{R}$.

Same idea applies to $\widetilde{A}_1$, $\widetilde{B}_1$. Then

$$Q = G_1 G_2 \cdots G_{n-2}$$

simultaneously tridiagonalizes (A, B).

Constructing G

How to construct $G \in \mathbb{R}^{\ell\times\ell}$ such that

$$G^T e_1 = e_1,\ G^T A G = \begin{bmatrix} \kappa & \tau e_1^T \\ \tau e_1 & \widetilde{A} \end{bmatrix},\ G^T B G = \begin{bmatrix} \mu & \sigma e_1^T \\ \sigma e_1 & \widetilde{B} \end{bmatrix}? \quad (\star)$$

Let $L = I + xy^T$ such that

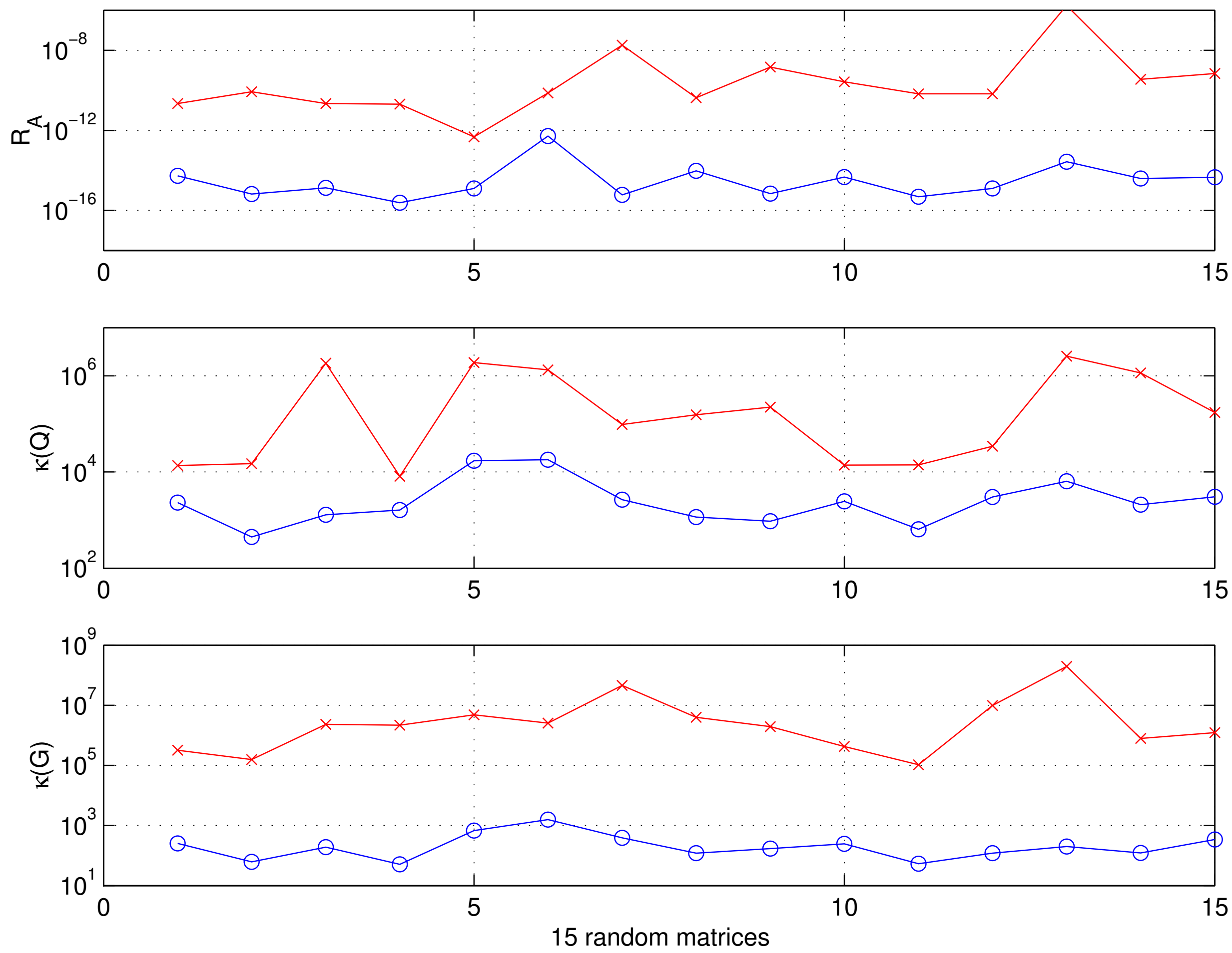
$$e_1^T L = e_1^T, \quad V^T(L^T K L)e_1 = \widetilde{\kappa} w, \quad V^T(L^T M L)e_1 = \widetilde{\mu} w,$$

where $V = [e_2, e_3, \ldots, e_\ell] \in \mathbb{R}^{\ell\times(\ell-1)}$, $\widetilde{\kappa}, \widetilde{\mu} \in \mathbb{R}$.
$w \in \mathbb{R}^{\ell-1}$: free parameter vector.

Then $\quad G = L \begin{bmatrix} 1 & 0 \\ 0 & H \end{bmatrix}, \quad H$: Householder re¤ector, satis£es $(\star)$

Numerical Experiments

- '-×-': tridiagonalization using $G = L$ with $L = I + xy^T$.
- '-o-': tridiagonalization using $G = LH$ with H: Householder matrix and $\kappa(L)$ minimal.



$$R_A = \frac{\|Q^T AQ - T\|_2}{\|A\|_2 \|Q\|_2}$$

$$\kappa(G) = \max_k \kappa(G_k)$$

Reduction to Tridiagonal-Diagonal Form

- First step in most eigensystem computations.
- Most compact form obtainable in a £nite number of steps.

Consists of two stages:

- Reduction to symmetric-diagonal form,

$$M^T(A-\lambda B)M = C - \lambda J.$$

- Reduction to tridiagonal-diagonal form,

$$Q^T(C-\lambda J)Q = T - \lambda \widetilde{J}.$$

J, $\widetilde{J}$: signature matrices with ± 1 on the diagonal.

Symmetric-Diagonal Reduction

- Block LDL^T factorization of B

$$P^T B P = LDL^T.$$

P: permutation matrix, L unit lower triangular.
D: diagonal with 1×1 or 2×2 blocks.

- Eigendecomposition of D:

$$D = X|\Lambda|^{1/2} J |\Lambda|^{1/2} X^T, \quad J \in \mathrm{diag}_q^n(\pm 1).$$

X: orthogonal, Λ: diag. matrix of eigenvalues.

$$\begin{aligned} M^{-1}(A - \lambda B)M^{-T} &= C - \lambda J, \\ M &= PLX|\Lambda|^{1/2}. \end{aligned}$$

Tridiagonal-Diagonal Reduction

$$Q^T C Q = T, \qquad Q^T J Q = \widetilde{J}.$$

- Reduction by uni£ed rotations.
- Reduction by uni£ed Householder re¤ectors.
- Reduction by mix of Householder re¤ectors & hyperbolic rotations.

Uni£ed Rotation

$$G = \begin{bmatrix} c & \gamma s \\ -s & c \end{bmatrix} \in \mathbb{R}^{2\times 2}, \quad c^2 + \gamma s^2 = \pm 1, \quad \gamma = J_{11}/J_{22},$$

$$G^T J G = \widetilde{J}, \quad Gx = \alpha e_1.$$

- $J = \pm I$: G is a Givens rotation.
- $J \neq \pm I$: G is a *hyperbolic rotation*.

For hyperbolic rotations,

$$\kappa_2(G) = \frac{|c| + |s|}{||c| - |s||}.$$

Condition number can be arbitrarily large.

Reduction by Uni£ed Rotation

$$C = \begin{bmatrix} \times & \times & 0 & 0 & 0 \\ \times & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & \times & \times & \times & \times \\ 0 & * & \times & \times & \times \end{bmatrix}, \quad J = \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \\ 1 \\ 1 \\ -1 \end{bmatrix}.$$

- Choose plane of rotation so that $\kappa(G)$ is minimized.
  - Reduce # hyp. rots used in the reduction.
  - Reduce risk of 2 hyp. rots acting in same plane.
- Apply uni£ed rotations implicitly.

Uni£ed Householder Re¤ectors

$$H = P\left(J - \frac{2vv^T}{v^T J v}\right), \qquad v^T J v \neq 0.$$

For any x s.t. $x^T J x \neq 0$, permutation P and v chosen s.t.

$$Hx = \alpha e_1.$$

H is $(\widetilde{J}, J)$-orthogonal, $\widetilde{J} = PJP$.

$$\sigma_{\min}^{-1}(H) = \sigma_{\max}(H) = \frac{v^T v}{|v^T J v|} + \sqrt{\left(\frac{v^T v}{v^T J v}\right)^2 - 1}.$$

Condition number can be arbitrarily large.

Reduction by Uni£ed Householder Re¤ectors

Similar to Householder tridiagonalization of symmetric matrix.

- ▶ Choose P s.t. $\kappa_2(H)$ is minimized.
- ▶ Product Hy performed implicitly:

$$Hy = P\Big(Jy - \frac{2v^T y}{v^T J v} v\Big).$$

- Twice less expensive than reduction via uni£ed rotations.
- Not clear which one has better numerical properties.

Mix Householder Re¤ector/Hyperbolic Rotations

Assume $J = \mathrm{diag}(I_p, -I_q)$ and let $x = (x_p^T, x_q^T)^T$.

- H_p, H_q: householder re¤ectors s.t.

$$H_p x_p = \alpha_p e_1, \qquad H_q x_q = \alpha_q e_1.$$

- G: hyperbolic rotation s.t. $G \begin{bmatrix} \alpha_p \\ \alpha_q \end{bmatrix} = \alpha e_1$.

Then

$$S = G \begin{bmatrix} H_p & 0 \\ 0 & H_q \end{bmatrix}, \qquad Sx = \alpha e_1.$$

Can show that

$$\kappa_2(S) \leq \kappa_2(H).$$

Numerical Experiments

- trd_ur: tridiagonalization by uni£ed rotations.
- trd_BG: Brebner & Grad's pseudosymmetric Givens reduction.

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C = randn(n); C = C+C'; J = sign(randn(n));
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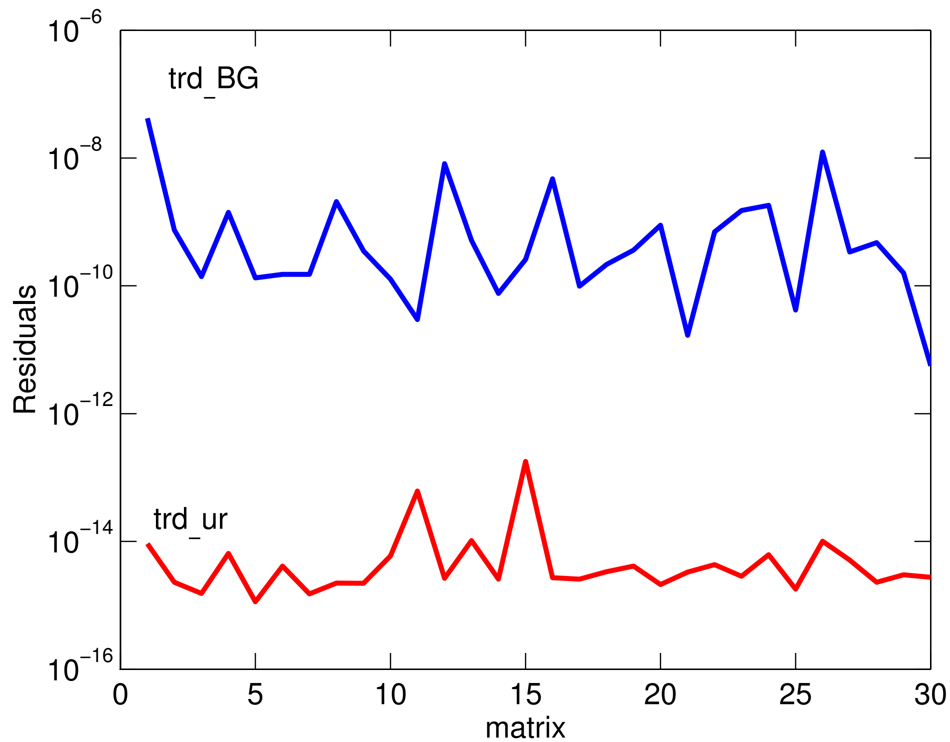

Residual

$$\mathcal{R} = \frac{\|Q^T C Q - T\|_2}{\|C\|_2 \|Q\|_2}$$

Direct/Implicit Application of Rotations

How hyperbolic rotation are applied to a matrix can be crucial to the stability of the reduction.

5×5 pair (C, J) generated by `mdsmax`.

$\kappa_2(Q) = 3.02$, $\kappa_{\max}(G) = 2 \times 10^3$

$$\mathcal{R} = \frac{\|Q^T C Q - T\|_2}{\|C\|_2 \|Q\|_2}, \qquad \mathcal{E} = \max_{i=1:n} \frac{|\lambda_i - \tilde{\lambda}_i|}{|\lambda_i|}.$$

$\mathcal{R}_{direct}$	$\mathcal{R}_{implicit}$	$\mathcal{E}_{direct}$	$\mathcal{E}_{implicit}$	$\mathrm{cond}(\lambda)$
5×10^{-12}	4×10^{-15}	4×10^{-10}	2×10^{-13}	4×10^2

Comparison Between Three Reductions

- `trd_ur`: tridiag. by uni£ed rotations
- `trd_uh`: tridiag. by uni£ed Householder re¤ectors.
- `trd_hr`: tridiag. by mixed Householder/hyp. rot.

300 matrices from `randn`, `randsvd`, `randjorth`.

- ▶ 85% of the time, all residuals are equivalent.
- ▶ `trd_uh` appears the least stable.
- ▶ Residual means: $\mathcal{R}_{ur} \approx \mathcal{R}_{hr} = O(10^{-15})$, $\mathcal{R}_{uh} = O(10^{-14})$.

Can generate matrices s.t. $\mathcal{R}_{ur} \gg \mathcal{R}_{hr}$ but harder for the converse.

Eigensolvers for Tridiagonal-Diagonal Pencils

Assume symm. indef. (A, B) reduced to tridiag.-diag. form (T, J).

- HZ algorithm [F.T, M. Berhanu]
  Related to HR alg. (*Brebner & Grad, Bunse-Gerstner*)
  HZ iteration driven by polynomial p:

  $$\widehat{T} = H^{-1}TH^{-T}, \quad \widehat{J} = H^{-1}JH^{-T},$$

  where $p(TJ) = HR$ (HR factorization).

- Aberth's iteration [D. Bini, L. Gemignani, F. T.]

  $$\lambda_j^{(k+1)} = \lambda_j^{(k)} - \frac{\zeta(\lambda_j^{(k)})}{1 - \zeta(\lambda_j^{(k)}) \sum_{\substack{k=1 \\ k \neq j}}^{m} (\lambda_j^{(k)} - \lambda_k^{(k)})^{-1}}, \; j = 1\colon m,$$

  where $\zeta(\lambda) = p(\lambda)/p'(\lambda) = \mathrm{trace}\big((TJ - \lambda I)^{-1}\big)$.

Structure Preserving Transformation

Consider $Q(\lambda) = \lambda^2 M + \lambda C + K$ and the symmetric linearization

$$A = \begin{bmatrix} 0 & K \\ K & C \end{bmatrix}, \quad B = \begin{bmatrix} K & 0 \\ 0 & -M \end{bmatrix}.$$

For QEP with nondefective λ, $\exists\ \mathcal{W}$ real nonsingular s.t.

$$\mathcal{W}^T A \mathcal{W} = \begin{bmatrix} 0 & D_K \\ D_K & D_C \end{bmatrix}, \quad \mathcal{W}^T B \mathcal{W} = \begin{bmatrix} D_K & 0 \\ 0 & -D_M \end{bmatrix},$$

with D_K, D_C and D_M real diagonal. [Garvey et al., 2001].

$(\widetilde{A}, \widetilde{B}) = \mathcal{W}^T (A, B) \mathcal{W}$ is symm. linearization of $\lambda^2 D_M + \lambda D_C + D_K$ with diagonal coeff. matrices.

Structure Preserving Algorithms

Work in progress.

- Jacobi-like algorithm. [S. Mackey & N. Mackey, F.T.]
  Make use of Clifford algebra.
- Reduction of blocks to tridiagonal form. [S. Garvey, N.J. Higham, F.T.]

$$\mathcal{W}^T A \mathcal{W} = \begin{bmatrix} 0 & T_K \\ T_K & T_D \end{bmatrix}, \quad \mathcal{W}^T B \mathcal{W} = \begin{bmatrix} T_K & 0 \\ 0 & -T_M \end{bmatrix},$$

where T_K, T_D and T_M are tridiagonal.
Eigenvalues of $\lambda^2 T_M + \lambda T_C + T_K$ via Aberth's iterations.

Summary

- Symmetric QEPs occur in several applications.
- Many interesting mathematical properties.
- Need for symmetry preserving numerical methods and software.
- New reductions to tridiagonal and tridiagonal-diagonal forms.
- New and improved eigensolvers for symmetric inde£nite pairs (T, J).
- Towards structure preserving algorithms.

Papers and reports:

`http://www.ma.man.ac.uk/~ftisseur/`