MANCHESTER 1824

The University of Manchester

A Reliable Algorithm for the Complete Solution of Quadratic Eigenvalue Problems

Françoise Tisseur
School of Mathematics
The University of Manchester

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

Joint work with Sven Hammarling and Christopher Munro.

Eigensolvers for QEPs

$$Q(\lambda) = \lambda^2 A_2 + \lambda A_1 + A_0, \quad A_i \in \mathbb{C}^{n\times n}$$

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

- Eigensolver often absent from numerical libraries.
- Commonly solved by linearization.
  - Convert $Q(\lambda)$ into linear pencil $\mathcal{A} - \lambda B$, e.g.,

$$\begin{bmatrix} A_0 & 0 \\ 0 & I \end{bmatrix} - \lambda \begin{bmatrix} -A_1 & -A_2 \\ I & 0 \end{bmatrix} = \mathcal{A} - \lambda\mathcal{B}.$$

  - Solve generalized eigenvalue problem (GEP).
  - Recover eigenvectors of $Q(\lambda)$ from those of $\mathcal{A} - \lambda\mathcal{B}$.

Numerical Issues

- **Infinitely many linearizations** to choose from.
- Solving QEPs with a backward stable alg. (e.g., QZ alg.) applied to a linearization can be **backward unstable** for the QEP.
- Linearizations can have **widely varying eigenvalue condition numbers**.
- Many QEPs have singular A_0 and/or A_2.

Numerical solution of QEPs requires special attention.

Objectives

- To design a general purpose eigensolver for dense QEPs—**`quadeig`**.
- Incorporate:
  - Appropriate choice of linearization.
  - Deflation of 0 and ∞ eigenvalues.
  - Eigenvalue parameter scaling.
  - Advantageous use of block structure.
  - Careful recovery of the eigenvectors
- A MATLAB and Fortran implementation.

Choice of Linearization

Opt for **a companion form** $C(\lambda) = \mathcal{A} - \lambda\mathcal{B}$.

- Simple block structure.
- Always a linearization, i.e, there exist $E(\lambda)$ and $F(\lambda)$ with constant, nonzero determinants s.t.

$$\begin{bmatrix} Q(\lambda) & 0 \\ 0 & I \end{bmatrix} = E(\lambda)C(\lambda)F(\lambda).$$

- Left/right e'vecs of $Q(\lambda)$ are easily recovered from those of companion linearizations.
- "Good" backward error and conditioning properties when $\|A_2\|_2 \approx 1$, $i = 0\colon 2$.

Companion Forms $C_i(\lambda) = \mathcal{A}_i - \lambda\mathcal{B}_i$

i	$\mathcal{A}_i$	$-\mathcal{B}_i$	$\texttt{eig}(\mathcal{A}_i, \mathcal{B}_i)$[1]	$\texttt{eig}(\mathcal{A}_i, \mathcal{B}_i)$[2]
1	$\begin{bmatrix} A_1 & A_0 \\ -I & 0 \end{bmatrix}$	$\begin{bmatrix} A_2 & 0 \\ 0 & I \end{bmatrix}$	100 s	99 s
2	$\begin{bmatrix} A_1 & -I \\ A_0 & 0 \end{bmatrix}$	$\begin{bmatrix} A_2 & 0 \\ 0 & I \end{bmatrix}$	100 s	101 s
3	$\begin{bmatrix} A_0 & 0 \\ 0 & I \end{bmatrix}$	$\begin{bmatrix} A_1 & A_2 \\ -I & 0 \end{bmatrix}$	139 s	145 s
4	$\begin{bmatrix} A_0 & 0 \\ 0 & I \end{bmatrix}$	$\begin{bmatrix} A_1 & -I \\ A_2 & 0 \end{bmatrix}$	140 s	145 s
$\vdots$	$\vdots$	$\vdots$		

[1] A_2 random diagonal, A_0, A_1 random tridiagonal, $n = 1000$.
[2] A_2 random upper triangular, A_0, A_1 random, full, $n = 1000$.

Companion Forms $C_i(\lambda) = \mathcal{A}_i - \lambda \mathcal{B}_i$ (cont.)

i	$\mathcal{A}_i$	$-\mathcal{B}_i$	
1	$\begin{bmatrix} A_1 & A_0 \\ -I & 0 \end{bmatrix}$	$\begin{bmatrix} A_2 & 0 \\ 0 & I \end{bmatrix}$	
2	$\begin{bmatrix} A_1 & -I \\ A_0 & 0 \end{bmatrix}$	$\begin{bmatrix} A_2 & 0 \\ 0 & I \end{bmatrix}$	$\rightarrow$ used by **quadeig**.
3	$\begin{bmatrix} A_0 & 0 \\ 0 & I \end{bmatrix}$	$\begin{bmatrix} A_1 & A_2 \\ -I & 0 \end{bmatrix}$	$\rightarrow$ used by **polyeig**.
4	$\begin{bmatrix} A_0 & 0 \\ 0 & I \end{bmatrix}$	$\begin{bmatrix} A_1 & -I \\ A_2 & 0 \end{bmatrix}$	

- $\mathcal{B}_1$, $\mathcal{B}_2$ are block diagonal.
- Deflation easy to implement on C_2—to be discussed.

Eigenvector Relations for C_2

Identify λ with (α, β) ($|\alpha|^2 + |\beta|^2 = 1$) for which $\lambda = \alpha/\beta$.

$Q(\alpha, \beta) = \alpha^2 A_2 + \alpha\beta A_1 + \beta^2 A_0, \quad Q(\alpha, \beta)x = 0,\ y^* Q(\alpha, \beta),$

$C_2(\alpha, \beta) = \beta\left[\begin{smallmatrix} A_1 & -I \\ A_0 & 0 \end{smallmatrix}\right] + \alpha\left[\begin{smallmatrix} A_2 & 0 \\ 0 & I \end{smallmatrix}\right],\ C_2(\alpha, \beta)z = 0,\ w^* C_2(\alpha, \beta) = 0.$

Left/right e'vecs of Q easily recovered from those of C_2:

$$w = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \begin{bmatrix} \alpha y \\ \beta y \end{bmatrix}, \quad z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{cases} \begin{bmatrix} \alpha x \\ -\beta A_0 x \end{bmatrix} & \text{if } \alpha \neq 0, \\ \begin{bmatrix} \beta x \\ \beta A_1 x \end{bmatrix} & \text{if } \alpha = 0. \end{cases}$$

Backward Errors and Conditioning

$\kappa_L(\alpha,\beta)$: e'val condition number for (α,β) as e'val of L.

$\eta_L(x,\alpha,\beta)$: b'err for approximate right eigenpair (x,α,β).

$\eta_L(y^*,\alpha,\beta)$: b'err for approximate left eigenpair (y,α,β).

Can show that $\kappa_Q(\alpha,\beta) \approx \kappa_{C_2}(\alpha,\beta)$ and

$$\eta_Q(z_1,\alpha,\beta) \approx \eta_{C_2}(z,\alpha,\beta), \qquad \eta_Q(w_k^*,\alpha,\beta) \approx \eta_{C_2}(w^*,\alpha,\beta),$$

for some $k \in \{1,2\}$ and all e'vals (α,β) if

$$\frac{\max(1,\max_{i=0:2}\|A_i\|_2)^2}{|\alpha|^2\|A_2\|_2 + |\alpha||\beta|\|A_1\|_2 + |\beta|^2\|A_0\|_2} \approx 1.$$

Eigenvalue Parameter Scaling

Let $\lambda = \mu\gamma$, $\gamma \neq 0$ and convert $Q(\lambda) = \lambda^2 A_2 + \lambda A_1 + A_0$ to

$$\begin{aligned} \delta Q(\mu\gamma) &= \mu^2(\delta\gamma^2 A_2) + \mu(\delta\gamma A_1) + \delta A_0 \\ &= \mu^2 \widetilde{A}_2 + \mu \widetilde{A}_1 + \widetilde{A}_0 =: \widetilde{Q}(\mu). \end{aligned}$$

- $\eta_Q(x, \alpha, \beta) = \eta_{\widetilde{Q}}(x, \widetilde{\alpha}, \widetilde{\beta})$.
- Fan, Lin and Van Dooren scaling (2004).
- Tropical scaling: Gaubert and Sharify (2009).

Fan, Lin and Van Dooren Scaling

If $\|A_0\|_2, \|A_2\|_2 \neq 0$, then $\gamma = \sqrt{\frac{\|A_0\|_2}{\|A_2\|_2}}, \; \delta = \frac{2}{\|A_0\|_2 + \|A_1\|_2 \gamma}$

minimize the maximum distance

$$\min_{\gamma,\delta} \max\{\| \underbrace{\delta A_0}_{\widetilde{A}_0} \|_2 - 1, \| \underbrace{\delta\gamma A_1}_{\widetilde{A}_1} \|_2 - 1, \| \underbrace{\delta\gamma^2 A_2}_{\widetilde{A}_2} \|_2 - 1\}.$$

Can show that if $\|A_1\|_2 \leq (\|A_2\|_2 \|A_0\|_2)^{1/2}$ or $|\lambda| = O(\gamma)$ then with this scaling,

$$\eta_{\widetilde{Q}} \approx \eta_{\widetilde{C}_2}, \qquad \kappa_{\widetilde{Q}} \approx \kappa_{\widetilde{C}_2}.$$

Tropical Scaling – Gaubert & Sharify

γ chosen as tropical roots of max-times scalar quadratic

$$q_{\mathrm{trop}}(\gamma) = \max(\|A_2\|_2\gamma^2, \|A_1\|_2\gamma, \|A_0\|_2)$$

and $\delta = q_{\mathrm{trop}}(\gamma)$.

- If $\|A_1\|_2 \le (\|A_2\|_2\|A_0\|_2)^{1/2}$, one double tropical root $\gamma = (\|A_0\|_2/\|A_2\|_2)^{1/2}$ (same as Fan, Lin, Van Dooren).
- Otherwise, two distinct tropical roots

$$\gamma^+ = \|A_1\|_2/\|A_2\|_2, \quad \gamma^- = \|A_0\|_2/\|A_1\|_2, \quad (\gamma^+ > \gamma^-).$$

Then $\eta_{\widetilde{Q}} \approx \eta_{\widetilde{C}_2}$, $\kappa_{\widetilde{Q}} \approx \kappa_{\widetilde{C}_2}$ if $\begin{cases} \gamma = \gamma^+ \text{ and } |\lambda| \ge \gamma, \\ \gamma = \gamma^- \text{ and } |\lambda| \le \gamma. \end{cases}$

0 and ∞ Eigenvalues

- $r_0 = \text{rank}(A_0) < n \;\Rightarrow\;$ Q has at least $n - r_0$ zero e'vals.
- $r_2 = \text{rank}(A_2) < n \;\Rightarrow\;$ Q has at least $n - r_2$ ∞ e'vals.

For example,

$$Q(\lambda) = \lambda^2 \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} + \lambda \begin{bmatrix} 0 & 1 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}$$

has e'vals $\{0, 0, -1, \infty\}$.

- Right e'vecs of Q with e'vals 0 generate right nullspace of A_0.
- Left e'vecs of Q with e'vals ∞ generate left nullspace of A_2.

Rank Determination

- **quadeig** computes rank(A_0) and rank(A_2), and deflates 0 and/or ∞ e'vals if needed.
- QR factorizations with column pivoting:

$$Q_i^* A_i P_i = \begin{array}{c} \\ k \\ n-r_i \end{array} \!\!\begin{array}{c} \begin{array}{cc} r_i & n-r_i \end{array} \\ \begin{bmatrix} R_{11}^{(i)} & R_{12}^{(i)} \\ 0 & 0 \end{bmatrix} \end{array}, \quad i = 0, 2.$$

- Can overestimate the rank $\Rightarrow$ may deflate fewer e'vals than could have done.

Block Triangularization of C_2

Transform $C_2(\lambda) = \left[\begin{smallmatrix} A_1 & -I \\ A_0 & 0 \end{smallmatrix}\right] - \lambda \left[\begin{smallmatrix} -A_2 & 0 \\ 0 & -I \end{smallmatrix}\right]$ into

$$\begin{bmatrix} S_{11} & S_{12} & S_{13} \\ 0 & S_{22} & S_{23} \\ 0 & 0 & 0_{n-r_0} \end{bmatrix} - \lambda \begin{bmatrix} T_{11} & T_{12} & T_{13} \\ 0 & 0_{n-r_2} & T_{23} \\ 0 & 0 & I_{n-r_0} \end{bmatrix},$$

where $r_i = \operatorname{rank}(A_i)$, $i = 0, 2$.

- 2 QR fact with col piv and 1 COD if $r_0 < n$ and $r_2 < n$.
- Make use of block structure of $C_2(\lambda)$.
- Call QZ on $S_{11} - \lambda T_{11}$, with T_{11} usually upper triang.
- $Q(\lambda)$ nonregular if S_{22} singular.
- Cost of deflation negligible compared with overall cost.

Right Eigenvector Recovery

- **Non-deflated e'vals**: recover e'vec x of Q from e'vec of C_2, $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} \alpha x \\ -\beta A_0 x \end{bmatrix}$ if $\alpha \neq 0$, and $\begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \begin{bmatrix} \beta x \\ \beta A_1 x \end{bmatrix}$ if $\alpha = 0$.
  - If $\|A_1\| \leq (\|A_2\|\|A_0\|)^{1/2}$ or $\det A_0 = 0$ then $x = z_1$.
  - Otherwise, take for x the vector z_1 or $A_0^{-1} z_2$ with smallest backward error.
- **Deflated e'vals**. Use COD of A_i, $i = 1, 2$,

$$Q_i^* A_i Z_i = \begin{array}{c} \\ r_i \\ n-r_i \end{array} \begin{array}{c} \begin{array}{cc} r_i & n-r_i \end{array} \\ \begin{bmatrix} T_{11} & 0 \\ 0 & 0 \end{bmatrix} \end{array}.$$

  - Last $n - r_0$ cols. of Z_0 are e'vecs with e'val 0.
  - Last $n - r_2$ cols. of Z_2 are e'vecs with e'val ∞.

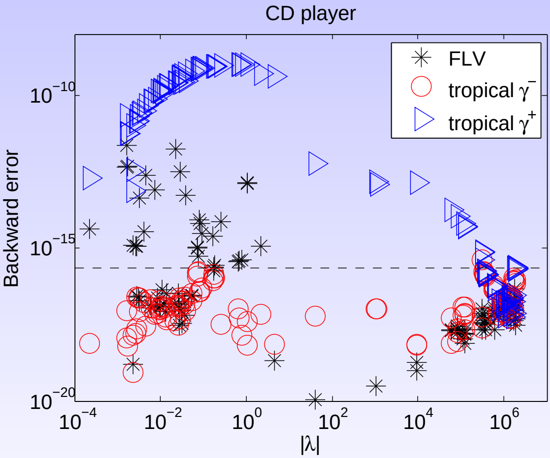
QEPs from NLEVP Collection

Problem	n	τ_Q	`polyeig` $\eta_Q(x,\lambda)$	`quadeig` $\eta_Q(x,\lambda)$	`quadeig` $\eta_Q(y^*,\lambda)$
`power_plant`	8	7-e1	1e-8	4e-16	5e-17
`hospital`	24	7e-2	3e-13	6e-16	6e-16
`cd_player`	60	9e+3	2e-10	2e-12	5e-12
`speaker_box`	107	2e-5	3e-11	5e-16	5e-16
`damped_beam`	200	2e-4	3e-9	9e-16	1e-15
`shaft`	400	1e-6	9e-8	9e-16	6e-16
`railtrack`	1005	2e1	2e-8	2e-15	8e-15

Fan, Lin, Van Dooren scaling (default).

`quadeig` **backward stable** for $\tau_Q = \|A_1\|/\sqrt{\|A_2\|\|A_0\|} \lesssim 1$.

Tropical Scaling for CD_player QEP



Tropical roots: $\gamma^- = 2.8 \times 10^{-2}, \;\; \gamma^+ = 2.5 \times 10^{6}$.

Some Timings

Problem	n	polyeig Λ	polyeig (Λ, X)	quadeig$^{(*)}$ Λ	quadeig$^{(*)}$ (Λ, X)
acoustic_wave_2D	870	117s	253s	115s	191s
damped_beam	1000	92s	240s	97s	163s
spring	1000	203s	323s	92s	201s
railtrack	1005	17s	69s	5s	6s
railtrack2	1410	128s	303s	79s	113s

railtrack(2): QEPs with singular A_2, A_0.

$(*)$: uses the MATLAB NAG Toolbox.

Concluding Remarks

- **quadeig** is backward stable for heavily damped problems.
- Deflation strategy can produce significant speedups.
- Returns e'vals and optionally right & left e'vecs, e'val condition numbers, backward errors of right/left approx. eigenpairs.
- Faster & more stable than **polyeig**.
- MATLAB and Fortran implementations.

For papers and Eprints,
`http://www.ma.man.ac.uk/~ftisseur/`