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An Algorithm for the Complete Solution of Quadratic Eigenvalue Problems

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Joint work with Sven Hammarling and Christopher Munro.

Quadratic Eigenvalue Problem (QEP)

Consider $Q(\lambda) = \lambda^2 M + \lambda D + K \in \mathbb{C}[\lambda]^{n \times n}$.

Assume $Q(\lambda)$ regular ($\det(Q(\lambda)) \not\equiv 0$).

QEP: find nonzero vectors x, y and scalars $\lambda \in \mathbb{C}$ s.t.

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

- $Q(\lambda)$ has $2n$ **e'vals**. Finite e'vals are roots of $\det(Q(\lambda)) = 0$.
- E'val at 0 when K is singular and e'val at ∞ when M is singular.

Example 1

$$Q(\lambda) = \lambda^2 \begin{bmatrix} 0 & 8 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \lambda \begin{bmatrix} 1 & -6 & 0 \\ 2 & -7 & 0 \\ 0 & 0 & 0 \end{bmatrix} + \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Regular: $\det Q(\lambda) = -6\lambda^5 + 11\lambda^4 - 12\lambda^3 + 12\lambda^2 - 6\lambda + 1 \not\equiv 0.$

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

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

NLEVP Toolbox

Collection of Nonlinear Eigenvalue Problems : T. Betcke, N. J. Higham, V. Mehrmann, C. Schröder, F. T., 2011.

- Quadratic, polynomial, rational and other nonlinear eigenproblems.
- Provided in the form of a MATLAB Toolbox. Compatible with GNU Octave.
- Problems from real-life applications + specifically constructed problems.

http://www.mims.manchester.ac.uk/research/numerical-analysis/nlevp.html

Sample of Quadratic Problems

$n \times m$ quadratic $Q(\lambda) = \lambda^2 M + \lambda D + K$.

Speaker box (`pep,qep,real,symmetric`).
$n = m = 107$. Finite element model of a speaker box.
$\|M\|_2 = 1$, $\|D\|_2 = 5.7 \times 10^{-2}$, $\|K\|_2 = 1.0 \times 10^7$.

Railtrack (`pep,qep,t-palindromic,sparse`).
$n = m = 1005$. Model of vibration of rail tracks under the excitation of high speed trains. $M = K^T$, $D = D^T$.

Surveillance (`pep,qep,real,nonsquare, nonregular`). $n = 21$, $m = 16$. From calibration of surveillance camera using human body as calibration target.

Standard Solution Process

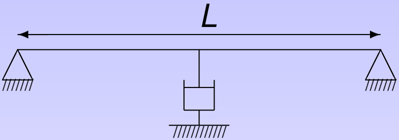
Find all λ and x satisfying $Q(\lambda)x = (\lambda^2 M + \lambda D + K)x = 0$.

- Commonly solved by linearization:
  - **Convert** $Q(\lambda)x = 0$ into $(\mathcal{A} - \lambda\mathcal{B})\xi = 0$, e.g.,

$$\mathcal{A} - \lambda\mathcal{B} = \begin{bmatrix} K & 0 \\ 0 & I \end{bmatrix} - \lambda \begin{bmatrix} -D & -M \\ I & 0 \end{bmatrix}, \quad \xi = \begin{bmatrix} x \\ \lambda x \end{bmatrix}.$$

  - **Solve** $(\mathcal{A} - \lambda\mathcal{B})\xi = 0$ with an eigensolver for generalized eigenproblem (e.g., QZ algorithm).
  - **Recover** eigenvectors of $Q(\lambda)$ from those of $\mathcal{A} - \lambda\mathcal{B}$.
- Eigensolver often **absent from numerical libraries**.

Beam Problem



- Transverse displacement $u(x,t)$ governed by

$$\rho A \frac{\partial^2 u}{\partial t^2} + c(x)\frac{\partial u}{\partial t} + EI\frac{\partial^4 u}{\partial x^4} = 0.$$

$$u(0,t) = u''(0,t) = u(L,t) = u''(L,t) = 0.$$

- Separation of variables $u(x,t) = e^{\lambda t} v(x,\lambda)$ yields the **eigenvalue problem for the free vibrations**:

$$\lambda^2 \rho A v(x,\lambda) + \lambda c(x) v(x,\lambda) + EI\frac{\partial^4}{\partial x^4} v(x,\lambda) = 0.$$

Discretized Beam Problem

Finite element method leads to

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

with **symmetric** $M, D, K \in \mathbb{R}^{n\times n}$. $M > 0$, $K > 0$, $D \geq 0$.

Roots of $x^* Q(\lambda) x = 0$, $x \in \mathbb{C}^n \setminus \{0\}$,

$$\lambda = \frac{-(x^* Dx) \pm \sqrt{(x^* Dx)^2 - 4(x^* Mx)(x^* Kx)}}{2(x^* Mx)}.$$

- $M > 0$, $K > 0$, $D \geq 0 \;\Rightarrow$ all e'vals have $\mathrm{Re}(\lambda) \leq 0$.
- D is rank 1. Can show n pure imaginary e'vals.

Eigenvalues of $Q(\lambda) = \lambda^2 M + \lambda D + K$

When M, K are nonsingular then theoretically

$$C_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} + \begin{bmatrix} D & K \\ -I & 0 \end{bmatrix},$$

$$L_1(\lambda) = \lambda \begin{bmatrix} M & 0 \\ 0 & -K \end{bmatrix} + \begin{bmatrix} D & K \\ K & 0 \end{bmatrix}, \quad L_2(\lambda) = \lambda \begin{bmatrix} 0 & M \\ M & D \end{bmatrix} + \begin{bmatrix} -M & 0 \\ 0 & K \end{bmatrix}$$

have the same eigenvalues as $Q(\lambda)$.

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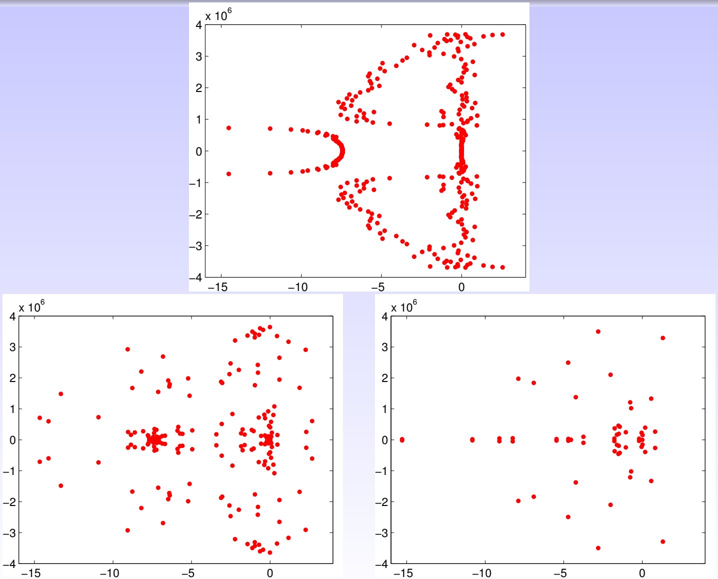
have the same eigenvalues as $Q(\lambda)$.

```
coeffs = nlevp('damped_beam',100);
K = coeffs{1}; D = coeffs{2}; M = coeffs{3};
I = eye(2*nele); O = zeros(2*nele);
eval = eig([D K; -I O],-[M O; O I]; % C1
%eval = eig([D K; K O],-[M O; O -K]; % L1
%eval = eig([-M O; O K],-[O M; M D]; % L2
plot(eval,'.r');
```

Computed Spectra of C_1, L_1 and L_2



Sensitivity and Stability of Linearizations

- **Condition number** measures sensitivity of the solution of a problem to perturbations in the data.
- **Backward error** measures how well the problem has been solved.

error in solution $\lesssim$ condition number $\times$ backward error.

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- **Condition number** measures sensitivity of the solution of a problem to perturbations in the data.
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error in solution $\lesssim$ condition number $\times$ backward error.

For a given $Q(\lambda)$, infinitely many linearizations exist:

- can have **widely varying eigenvalue condition numbers**,
- computed eigenpairs can have **widely varying backward errors**.

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.

Linearization for $Q(\lambda) = \lambda^2 M + \lambda D + K$

Opt for $C(\lambda) = \begin{bmatrix} D & -I \\ K & 0 \end{bmatrix} + \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix}$ **(companion form, Fiedler pencil)**

- 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.
- Deflation of 0 and ∞ e'vals easy to implement.
- "Good" backward error and conditioning properties.

Eigenvalue Condition Numbers $\kappa_Q(\lambda)$

$$Q(\lambda)x = 0, \quad y^*Q(\lambda) = 0, \quad \Delta Q(\lambda) = \lambda^2 \Delta M + \lambda \Delta D + \Delta K.$$

For λ **simple, nonzero and finite**,

$$\kappa_Q(\lambda) = \lim_{\epsilon \to 0} \sup \left\{ \frac{|\Delta\lambda|}{\epsilon|\lambda|} : \left[(Q + \Delta Q)(\lambda + \Delta\lambda)\right](x + \Delta x) = 0, \right.$$
$$\left. \|\Delta M\|_2 \le \epsilon\|M\|_2,\ \|\Delta D\|_2 \le \epsilon\|D\|_2,\ \|\Delta K\|_2 \le \epsilon\|K\|_2 \right\}.$$

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$$\left. \|\Delta M\|_2 \le \epsilon \|M\|_2,\ \|\Delta D\|_2 \le \epsilon \|D\|_2,\ \|\Delta K\|_2 \le \epsilon \|K\|_2 \right\}.$$

Can show that [T. 01]

$$\kappa_Q(\lambda) = \frac{\big(|\lambda|^2 \|M\|_2 + |\lambda| \|D\|_2 + \|K\|_2\big) \|y\|_2 \|x\|_2}{|\lambda| |y^*(2\lambda M + D)x|}.$$

When $\lambda = 0$ or ∞, use **homogeneous form** of Q.

Eigenvalue Condition Numbers $\kappa_Q(\alpha, \beta)$

Homogeneous form: $Q(\alpha, \beta) = \alpha^2 M + \alpha\beta D + \beta^2 K$.

E'vals are pairs $(\alpha, \beta) \neq (0, 0)$ s.t. $\det Q(\alpha, \beta) = 0$, $\lambda = \alpha/\beta$.

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For (α, β) simple with right/left e'vecs x, y, [Dedieu, T., 03]

$$\kappa_Q(\alpha, \beta) = \frac{\left(|\alpha|^4 \|M\|_2^2 + |\alpha|^2 |\beta|^2 \|D\|_2^2 + |\beta|^4 \|K\|_2^2\right)^{1/2} \|y\|_2 \|x\|_2}{\left| y^* (\bar{\beta} \mathcal{D}_\alpha Q - \bar{\alpha} \mathcal{D}_\beta Q)|_{(\alpha,\beta)} x \right|}.$$

Angle between original and perturbed eigenvalues satisfies

$$\left|\theta\big((\alpha, \beta), (\tilde{\alpha}, \tilde{\beta})\big)\right| \leq \kappa_Q(\alpha, \beta) \|\Delta Q\| + o(\|\Delta Q\|).$$

Here $\Delta Q = (\Delta M, \Delta D, \Delta K)$.

Similar expression for $\kappa_C(\alpha, \beta)$, $C(\lambda) = \begin{bmatrix} D & -I \\ K & 0 \end{bmatrix} + \lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix}$.

Eigenvalue Condition Numbers $\kappa_Q(\alpha,\beta)$

Homogeneous form: $Q(\alpha,\beta) = \alpha^2 M + \alpha\beta D + \beta^2 K$.

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For (α,β) simple with right/left e'vecs x, y, [Dedieu, T., 03]

$$\kappa_Q(\alpha,\beta) = \frac{\left(|\alpha|^4\|M\|_2^2 + |\alpha|^2|\beta|^2\|D\|_2^2 + |\beta|^4\|K\|_2^2\right)^{1/2}\|y\|_2\|x\|_2}{\left|y^*(\bar\beta\mathcal{D}_\alpha Q - \bar\alpha\mathcal{D}_\beta Q)|_{(\alpha,\beta)}x\right|}.$$

Angle between original and perturbed eigenvalues satisfies

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Similar expression for $\kappa_C(\alpha,\beta)$, $C(\lambda) = \left[\begin{smallmatrix} D & -I \\ K & 0 \end{smallmatrix}\right] + \lambda\left[\begin{smallmatrix} M & 0 \\ 0 & I \end{smallmatrix}\right]$.

Want $\kappa_Q(\alpha,\beta) \approx \kappa_C(\alpha,\beta)$ for all (α,β).

Backward Error $\eta_Q(x, \alpha, \beta)$

For an approximate (right) eigenpair (x, α, β) of $Q(\alpha, \beta)$,

$$\eta_Q(x, \alpha, \beta) = \min\{\, \epsilon : (Q(\alpha,\beta) + \Delta Q(\alpha,\beta))x = 0, \\ \|\Delta M\|_2 \le \epsilon \|M\|_2, \|\Delta D\|_2 \le \epsilon \|D\|_2, \|\Delta K\|_2 \le \epsilon \|K\|_2 \,\},$$

where $\Delta Q(\alpha,\beta) = \alpha^2 \Delta M + \alpha\beta \Delta D + \beta^2 \Delta K$.

Can show that [T.01]

$$\eta_Q(x, \alpha, \beta) = \frac{\|Q(\alpha,\beta)x\|_2}{\big(|\alpha|^2 \|M\|_2 + |\alpha||\beta| \|D\|_2 + |\beta|^2 \|K\|_2\big) \|x\|_2}.$$

Similar expression for $\eta_C(z, \alpha, \beta)$, $C(\lambda) = \left[\begin{smallmatrix} D & -I \\ K & 0 \end{smallmatrix}\right] + \lambda \left[\begin{smallmatrix} M & 0 \\ 0 & I \end{smallmatrix}\right]$.

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Similar expression for $\eta_C(z, \alpha, \beta)$, $C(\lambda) = \left[\begin{smallmatrix} D & -I \\ K & 0 \end{smallmatrix}\right] + \lambda\left[\begin{smallmatrix} M & 0 \\ 0 & I \end{smallmatrix}\right]$.
Want $\eta_Q(z_1, \alpha, \beta) \approx \eta_C(z, \alpha, \beta)$, $z = \left[\begin{smallmatrix} z_1 \\ z_2 \end{smallmatrix}\right]$.

Eigenvalue Parameter Scaling

Let $\lambda = \mu\gamma$, $\gamma \neq 0$ and convert $Q(\lambda) = \lambda^2 M + \lambda D + K$ to

$$\delta Q(\mu\gamma) = \mu^2(\gamma^2 \delta M) + \mu(\gamma\delta D) + \delta K = \mu^2 \widetilde{M} + \mu \widetilde{D} + \widetilde{K} =: \widetilde{Q}(\mu).$$

Choose γ such that

- the linearization process does not affect the eigenvalue condition numbers, i.e., $\kappa_Q(\alpha, \beta) \approx \kappa_C(\alpha, \beta)$ for all e'vals (α, β).
- the standard solution process in numerically stable, i.e., $\eta_Q(z_1, \alpha, \beta) \approx \eta_C(z, \alpha, \beta)$ for all e'vals (α, β), where $z = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix}$.

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Let $\lambda = \mu\gamma$, $\gamma \neq 0$ and convert $Q(\lambda) = \lambda^2 M + \lambda D + K$ to

$$\delta Q(\mu\gamma) = \mu^2(\gamma^2 \delta M) + \mu(\gamma\delta D) + \delta K = \boxed{\mu^2 \widetilde{M} + \mu \widetilde{D} + \widetilde{K} =: \widetilde{Q}(\mu)}.$$

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Try $\gamma = \exp(r)$, where r is a **tropical root** of a **tropical scalar quadratic** (proposed by Gaubert & Sharify, 09).

Tropical Scalar Polynomials

- Let $(\mathbb{R} \cup \{-\infty\}, \oplus, \otimes)$ be the **tropical semiring** with

$$a \oplus b = \max(a, b), \quad a \otimes b = a + b \quad \text{for all } a, b \in \mathbb{R} \cup \{-\infty\}.$$

- The piecewise affine function

$$p(x) = \bigoplus_{k=0}^{d} p_k \otimes x^{\otimes k} = \max_{0 \le k \le d} (p_k + kx), \quad p_k \in \mathbb{R} \cup \{-\infty\}$$

is a **tropical polynomial** of degree d.

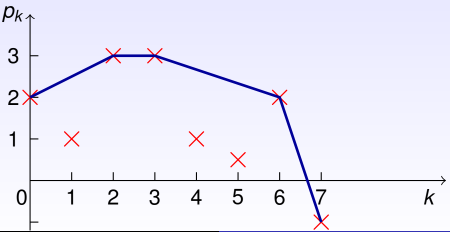
- The **tropical roots** of $p(x)$ are the points of nondifferentiability of $p(x)$.

Computation of Tropical Roots

Let $p(x) = \bigoplus_{k=0}^{d} p_k \otimes x^{\otimes k} = \max(p_0, p_1 + x, \ldots, p_d + dx)$.

- Upper boundary of **convex hull** of (k, p_k), $k = 0\colon d$.
- **Tropical roots** are minus the **slopes** of the segments (Legendre-Fenchel duality).
- Horizontal **width** of segment gives **multiplicity**.

$p(x) = max(2, 1+x, 3+2x, 3+3x, 1+4x, \frac{1}{2}+5x, 2+6x, -1+7x)$
has roots $-\frac{1}{2}, -\frac{1}{2}, 0, \frac{1}{3}, \frac{1}{3}, \frac{1}{3}, 3$.



Tropical Roots (cont.)

- Tropical roots can be computed in **linear time**.
- **Classical roots** of $p(x) = a_0 + a_1 x + \cdots + a_n x^n$ can be **bounded in terms of tropical roots** of $p_{\mathrm{trop}}(x) = \bigoplus_{k=0}^{d} p_k \otimes x^{\otimes k}$ (Sharify, 11).
- Let r_1, r_2 be the **tropical roots** of

  $$p_{\mathrm{trop}}(r) = \max(\log(\|K\|), \log(\|D\|) + r, \log(\|M\|) + 2r).$$

  When $r_1 \gg r_2$ and M, D, K are well conditioned, $e^{r_1} \approx |\lambda_{\max}(Q)|$ and $e^{r_2} \approx |\lambda_{\min}(Q)|$, where $Q(\lambda) = \lambda^2 M + \lambda D + K$ (Gaubert & Sharify, 09).

Tropical Scaling

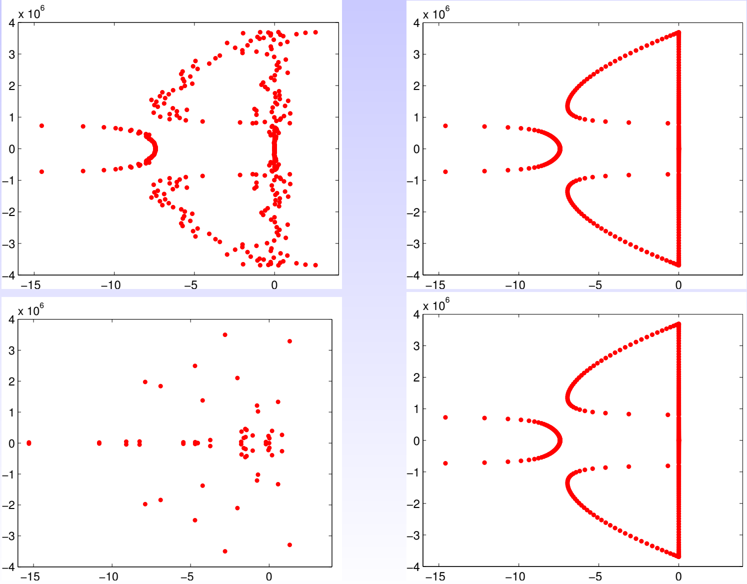
Let $p_{\text{trop}}(r) = \max(\log(\|K\|), \log(\|D\|) + r, \log(\|M\|) + 2r)$.

Convert $Q(\lambda)$ to $\delta Q(\mu\gamma)$, where

- $\gamma = e^{r}$, r is a tropical root of p_{trop},
- $\delta = e^{p_{\text{trop}}(r)}$.

- If $\|D\|_2^2 \le \|M\|_2\|K\|_2$ then $r_1 = r_2$ (one double root). Can show that $\eta_{\widetilde{Q}} \approx \eta_{\widetilde{C}}$, $\kappa_{\widetilde{Q}} \approx \kappa_{\widetilde{C}}$ for all e'vals.
- Otherwise, two distinct tropical roots $r_1 > r_2$. Can show that $\eta_{\widetilde{Q}} \approx \eta_{\widetilde{C}}$, $\kappa_{\widetilde{Q}} \approx \kappa_{\widetilde{C}}$ if $\begin{cases} r = r_1 \text{ and } |\lambda| \ge \gamma, \\ r = r_2 \text{ and } |\lambda| \le \gamma. \end{cases}$

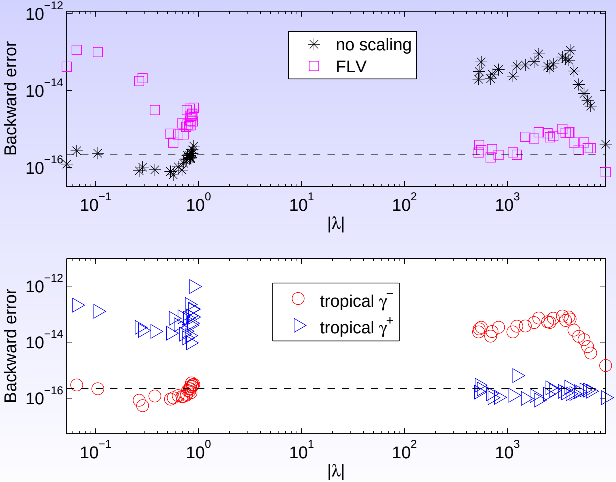
Beam Pb: $\Lambda(C), \Lambda(L_2)$ before/after Scaling



Modified Hospital Problem

Damping added s.t. $\|D\|_2^2 \gg \|M\|_2\|K\|_2$. $\gamma_{FLV} = \left(\frac{\|K\|_2}{\|M\|_2}\right)^{1/2} \approx 56.$

Two tropical roots: $\gamma^+ \approx 3.7 \times 10^3$ and $\gamma^- \approx 0.8$.



Deflation of 0 and ∞ eigenvalues

Transform $\widetilde{C}(\lambda) = \begin{bmatrix} \gamma\delta D & -I \\ \delta K & 0 \end{bmatrix} - \lambda \begin{bmatrix} -\gamma^2\delta M & 0 \\ 0 & -I \end{bmatrix}$ into

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

where $r_M = \text{rank}(M)$ and $r_K = \text{rank}(K)$.

- 2 QR fact with col piv and 1 COD if $r_M < n$ and $r_K < n$.
- Make use of block structure of $\widetilde{C}(\lambda)$.
- 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.

Some QEPs from NLEVP Collection

$\eta_Q(x, \lambda)$: backward error of computed eigenpair (x, λ).

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

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

Some Timings

Problem	n	polyeig Λ	polyeig (Λ, X)	quadeig Λ	quadeig (Λ, X)
acoustic_wave_2D	870	118s	202s	114s	191s
damped_beam	1000	92s	156s	97s	163s
spring	1000	182s	272s	94s	170s
railtrack2	1410	129s	306s	79s	113s

railtrack2: QEPs with singular M, K.

Extension to Higher Degree Polynomials

$$P(\lambda)x = (\lambda^\ell A_\ell + \cdots + \lambda A_1 + A_0)x = 0.$$

- Use **Fiedler linearization**:

$$F(\lambda) = \lambda \begin{bmatrix} A_\ell & & & & \\ & I & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & I \end{bmatrix} - \begin{bmatrix} -A_{\ell-1} & -A_{\ell-2} & \cdots & -A_1 & I \\ I & & & & \\ & \ddots & & & \\ & & I & & \\ & & & -A_0 & \end{bmatrix}.$$

Stability/conditioning similar to companion forms.

- Deflation of 0 and ∞ e'vals easy to implement.

- Work in progress: scaling strategy (Betcke's scaling, tropical roots, tropical eigenvalues, ...).

Summary

- **quadeig** is backward stable for not too heavily damped problems.
- Tropical mathematics useful for e'val scaling.
- Deflation strategy can produce significant speedups.
- Returns e'vals, right & left e'vecs, e'val condition numbers, b'errs of right/left approx. eigenpairs.
- MATLAB function available. Fortran implementation available soon.
- Extension to polynomial eigenproblem of degree $\ell > 2$.

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

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