A Review of Nonlinear Eigenvalue Problems

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Nonlinear Eigenvalue Problems (NEPs)

Let $F\colon \Omega \to \mathbb{C}^{n\times n}$ be a given matrix valued function.

The **nonlinear eigenvalue problem**: Find scalars λ and nonzero $x, y \in \mathbb{C}^n$ satisfying $F(\lambda)x = 0$ and $y^* F(\lambda) = 0$.

- λ is an e'val, x, y are corresponding right and left e'vecs.
- E'vals are solutions of $\det(F(\lambda)) = 0$.

In practice, elements of F most often **polynomial, rational or exponential functions of λ**.

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When F depends on e'vecs, see Jarlebring's talk, 11:00.

Comments

- NEPs underpin many areas of computational science and engineering.
- Collection of Nonlinear Eigenvalue Problems **NLEVP**, Betcke, Higham, Mehrmann, Schröder, T., 2011.
- NEPs can be very difficult to solve:
  - nonlinear,
  - large problem size,
  - poor conditioning,
  - lack of “good" numerical methods.
- Common feature of recent progress: clever conversion/approx. of $F(\lambda)x = 0$ by $(\mathcal{A} - \lambda\mathcal{B})\xi = 0$.

Polynomial Eigenvalue Problems (PEP)

Consider $n \times n$ matrix polynomial

$$P(\lambda) = \lambda^\ell A_\ell + \cdots + \lambda A_1 + A_0 \quad \text{(monomial form)}$$
$$= \phi_\ell(\lambda) P_\ell + \cdots + \phi_1(\lambda) P_1 + P_0 \quad \text{(non-monomial form)},$$

where $\phi_i(\lambda)$ is a polynomial of degree i.

- Assume $P(\lambda)$ is **regular**, i.e., $\det(P(\lambda)) \not\equiv 0$.
- $P(\lambda)$ has ℓn **e'vals**. Finites e'vals are roots of $\det(P(\lambda)) = 0$.
- Zero e'vals when $\det(A_0) = 0$ and ∞ e'vals when $\det(A_\ell) = 0$.

For theory, see Gohberg, Lancaster, Rodman, **Matrix Polynomials**, 1982 (Academic Press), 2009 (SIAM).

Schur's Theorem for Complex Matrices

Matrix version: if $A \in \mathbb{C}^{n\times n}$ then there exists a unitary U such that $U^*AU = T$ is a triangular matrix.

Subspaces version:

Theorem

Let $A \in \mathbb{C}^{n\times n}$. There are subspaces $\mathcal{V}_1, \dots, \mathcal{V}_n$ of $\mathbb{C}^n$ satisfying

(i) $\mathbb{C}^n = \mathcal{V}_1 \oplus \mathcal{V}_2 \oplus \cdots \oplus \mathcal{V}_n$,

(ii) *for $k = 1: n$, $\mathcal{V}_1 \oplus \cdots \oplus \mathcal{V}_k$, is A-invariant,*

(iii) *for $k = 1: n$, $\mathcal{V}_k = \langle u_k \rangle$, where $u_1, \dots u_n$ form an orthonormal system of vectors of $\mathbb{C}^n$.*

Schur-like Theorem for $Q(\lambda)$

Let $Q(\lambda) = \lambda^2 M + \lambda D + K$, $\det M \neq 0$.

Theorem (Zaballa, T., 2013)

Let $\lambda I - A \in \mathbb{C}[\lambda]^{2n\times 2n}$ be a linearization of $n \times n$ $Q(\lambda)$. There are subspaces $\mathcal{V}_1, \dots, \mathcal{V}_n$ of $\mathbb{C}^{2n}$ satisfying

(i) $\mathbb{C}^{2n} = \mathcal{V}_1 \oplus \mathcal{V}_2 \oplus \cdots \oplus \mathcal{V}_n$,

(ii) *for* $k = 1\colon n$, $\mathcal{V}_1 \oplus \cdots \oplus \mathcal{V}_k$ *is* A*-invariant,*

(iii) *for* $k = 1\colon n$, $\dim \mathcal{V}_k = 2$ *and* $\mathcal{V}_k = \langle u_k, Au_k \rangle$, *where* $u_1, \dots u_n$ *form an orthogonal system of vectors of* $\mathbb{C}^{2n}$.

- $\mathcal{V}_k = \langle u_k, Au_k \rangle$ is a **Krylov subspace** of dimension 2.
- The u_j are **generating vectors**.
- If $U = [u_1 \dots u_n]$ then $\mathcal{U} = [U \; AU]$ is nonsingular.

Schur-like Theorem: Matrix Form

Let $Q(\lambda) = \lambda^2 M + \lambda D + K \in \mathbb{C}[\lambda]^{n\times n}$ with $\det(M) \neq 0$.

Theorem (Zaballa, T., 2012)

For any linearization $\lambda I - A$ of $Q(\lambda)$, there exists $U \in \mathbb{C}^{2n\times n}$ with ***orthonormal columns*** *s.t. $[U\ AU]$ is nonsingular and*

$$[U\ AU]^{-1}A[U\ AU] = \begin{bmatrix} 0 & -T_0 \\ I_n & -T_1 \end{bmatrix},$$

where $I_n\lambda^2 + T_1\lambda + T_0$ is triangular and equivalent to $Q(\lambda)$.

- The columns of U are generating vectors for A.
- Extends to **arbitrary degree matrix polynomials**.
- **Issue: how to compute U?** No efficient way yet!

Standard Solution Process ($\ell = 2$)

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 $\mathcal{A} - \lambda\mathcal{B}$.
- Solution process extend to degree $\ell > 2$.
- Numerical issues with this process.

Numerical Issues

- **Infinitely many linearizations** to choose from.
  - Vector spaces of pencils $\mathbb{L}_1(P), \mathbb{L}_2(P), \mathbb{DL}(P)$, [$M^4$, 06], [Townsend, Nakatsukasa, Noferini, 12] (see Noferini's talk, today at 5:45).
  - Fiedler linearizations [Antoniou, Vologiannidis 04].
  - Linearizations for P expressed in polynomial bases [Amiraslani, Corless, Lancaster,09].

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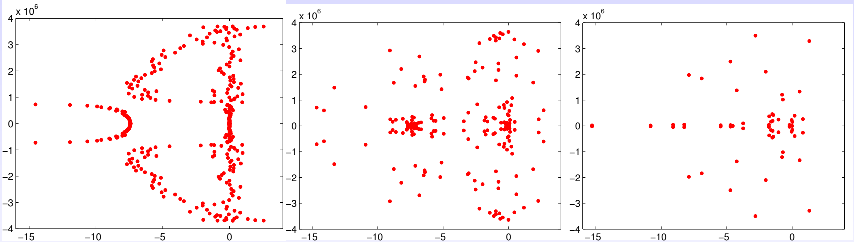
- Linearizations can have **widely varying eigenvalue condition numbers**.
- Solving PEPs with a backward stable alg. (e.g., QZ alg.) applied to a linearization can be **backward unstable** for the PEP.

Computed Spectra of C_1, L_1 and L_2

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

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



- Developed theory concerning the sensitivity and stability of linearizations [Higham, Mackey, T. 06, Higham, Li, T. 07, Grammont, Higham, T., 11].

Two Sided Factorizations

Suppose linearization L of P satisfies

$$L(\lambda)F(\lambda) = g \otimes P(\lambda), \qquad E(\lambda)L(\lambda) = h^T \otimes P(\lambda) \qquad (*)$$

with F, G of full rank and $g, h \in \mathbb{C}^\ell$.

$(*)$ Satisfied by most linearizations.

$(*)$ Yields relations between e'vecs for L & e'vecs for P:

- $z = F(\lambda)x \in \mathbb{C}^{\ell n}$ is a right e'vec of L with e'val λ iff $x \in \mathbb{C}^n$ is a right e'vec of P with e'val λ.
- If $w \in \mathbb{C}^{\ell n}$ is a left e'vec of L with e'val λ then $y = (g^* \otimes I_n)w \in \mathbb{C}^n$ is a left e'vec of P (if it's nonzero).

$(*)$ Implies $w^* L'(\lambda) z = y^* P'(\lambda) x$.

$(*)$ Relates residuals: $P(\lambda)x = E(\lambda)L(\lambda)z$.

Sensitivity and Stability of Linearizations

- Two sided factorizations allow analysis of growth factors $\kappa_L(\lambda)/\kappa_P(\lambda)$ (**conditioning**), $\eta_P(z_i, \lambda)/\eta_L(z, \lambda)$ (**backward error**).
- Importance of **scaling** QEPs/PEPs before computing e'vals via linearization.
  - Eigenvalue parameter scaling:

$$\lambda = \gamma\mu, \quad \widetilde{P}(\mu) := \delta P(\gamma\mu).$$

  - Does not affect sparsity of matrix coeffs.
  - γ, δ chosen to improve growth factors for conditioning and backward error.

`quadeig` for $Q(\lambda) = \lambda^2 M + \lambda D + K$.

- Eigensolver for dense (small to medium size) quadratics—**`quadeig`**.
- Incorporates:
  - Appropriate choice of linearization: uses $\begin{bmatrix} D & -I \\ K & 0 \end{bmatrix} - \lambda \begin{bmatrix} -M & 0 \\ 0 & -I \end{bmatrix}$.
  - Deflation of 0 and ∞ eigenvalues.
  - Eigenvalue parameter scaling (FLV/tropical). (see Sharify and Hook's talk, Tues., 4:45)
  - Careful recovery of the eigenvectors.
  - Backward stable when $\|D\| \lesssim (\|M\|\|K\|)^{1/2}$.
- MATLAB and Fortran implementations (NAG, LAPACK) [Hammarling, Munro, T. 2013].

Eigensolvers for Large Sparse QEPs

For $Q(\lambda) = \lambda^2 M + \lambda D + I$, they include:

- Q-Arnoldi method [Meerbergen, 08], $S = \begin{bmatrix} 0 & I \\ -M & -D \end{bmatrix}$.
  - Krylov subspace $\mathcal{K}_p(S, v) = \mathrm{span}\{v, Sv, \dots, S^p v\}$.
  - Use structure in Arnoldi iter. to save memory.
  - Can do implicit restart.
- Second Order Arnoldi (SOAR) [Bai & Su, 05].
  - 2nd order Krylov: $\mathcal{G}_p(D, M, b) = \mathrm{span}\{r_0, r_1, \dots, r_p\}$, $r_0 = b, r_1 = -Dr_0,\ r_j = -Dr_{j-1} - Mr_{j-2}$.
    If $v = \begin{bmatrix} b \\ 0 \end{bmatrix}$ then $\mathcal{G}_p$ defines $\mathcal{K}_p$.
  - $X_p^* Q(\lambda) X_p = \lambda^2 M_p + \lambda D_p + I_p$, $\mathrm{span} X_p = \mathcal{G}_p$.
  - Cannot do implicit restart.
- Two-level orthogonal Arnoldi (TOAR) [Su & Lu, 12].

Rational Eigenvalue Problems (REPs)

- Arise in a variety of physical applications, e.g.,
  - acoustic emissions of high speed trains,
  - band structure calculations for photonic crystals.

- Matrix function takes the form

$$R(\lambda) = P(\lambda) + \sum_{i=1}^{m} \frac{s_i(\lambda)}{q_i(\lambda)} E_i,$$

  - $P(\lambda)$ is a matrix polynomial,
  - s_i and q_i are scalar polynomials,
  - E_i are constant matrices.

In practice, m is small and $\text{rank}(E_i)$ is low.

Numerical Methods

$$R(\lambda) = P(\lambda) + \sum_{i=1}^{m} \frac{s_i(\lambda)}{q_i(\lambda)} E_i.$$

- Brute-force approach: turn the REP into a PEP.
  - Employed by practitioners.
  - Not practical when $q_i(\lambda)$ has several poles and $m \gg 1$.
- Treat the REP as a general nonlinear eigenproblem.
  - Limits the exploitation of the underlying structure and properties of the REP.
- **Linearizations** for rational problems .

Linearizations for Rational Problems

[Su & Bai, 11]

- Rewrite $R(\lambda) = P(\lambda) + \sum_{i=1}^{m} \frac{s_i(\lambda)}{q_i(\lambda)} E_i$ as

$$R(\lambda) = P(\lambda) + U(C - \lambda D)^{-1} V^*, \qquad (*)$$

  where U, V are $n \times r$. In practice $r \ll n \cdot \sum_{i=1}^{m} deg(q_i)$.

- Convert $(*)$ into linear pencil of dim. $nk + r$.

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Example: if $R(\lambda) = \lambda A + B + U(C - \lambda D)^{-1} V^*$ then $R(\lambda)x = 0$ is rewritten as a **linear eigenproblem**

$$\left(\lambda \begin{bmatrix} A & 0 \\ 0 & D \end{bmatrix} + \begin{bmatrix} B & U \\ V^* & -C \end{bmatrix}\right) \begin{bmatrix} x \\ (C - \lambda D)^{-1} V^* x \end{bmatrix} = 0.$$

Genuine Nonlinear Eigenproblems

$F(\lambda)x = 0$ with $F\colon \Omega \to \mathbb{C}^{n\times n}$, $\Omega \subseteq \mathbb{C}$.

Some applications:

- PDE models with λ-dependent boundary conditions or material conditions. E.g.,

$$F(\lambda) = K - \lambda M + i(\lambda - \sigma_1^2)^{\frac{1}{2}} W_1 + i(\lambda - \sigma_2^2)^{\frac{1}{2}} W_2 = 0$$

(model radio-frequency gun cavity, [Liao, 07]).

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- Characteristic function of delay differential eqns. E.g.,

  $$F(\lambda) = -\lambda I + A_1 + A_2 e^{-\tau\lambda} + A_3 \int_{-1}^{0} e^{\lambda s}(e^{(s+\frac{1}{2})^2} - e^{\frac{1}{4}})\, ds$$

  (delay-diff. eqn with distributed delays, [Jarlebring et al, 12]).

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  (delay-diff. eqn with distributed delays, [Jarlebring et al, 12]).

- Use of special basis functions in the discretization.

Methods for Nonlinear Eigenproblems

- Typically interested in only a few e'vals closest to a target point, a line or small region of complex plane.

- Numerical methods include
  - Newton methods, inverse iteration,. . . [Ruhe, 73].
  - Nonlinear Rayleigh-Ritz iterative procedure, e.g., nonlinear Arnoldi [Voss, 04], NRRIT, [Liao, Bai, Lee, Ko, 06], rational Krylov [Jarlebring, Voss, 05], Jacobi-Davidson [Voss, 04], ...
  - Contour integration [Beyn, Effenberger, Kressner, 11; Sakurai et al, 10]. (see Yamamoto's talk, Tues, 5:45)

Numerical Methods (Cont.)

- Approximate $F(\lambda)$ by a polynomial

$$F(\lambda) \approx P_d(\lambda) = a_0(\lambda)A_0 + a_1(\lambda)A_1 + \cdots + a_d(\lambda)A_d,$$

  with $a_j(\lambda)$, e.g., Taylor, Chebyshev, Newton, Hermite.

- Solve $P_d(\lambda)x = 0$ (see Karl Meebergen's talk).

Numerical Methods (Cont.)

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  with $a_j(\lambda)$, e.g., Taylor, Chebyshev, Newton, Hermite.

- Solve $P_d(\lambda)x = 0$ (see Karl Meebergen's talk).
  - Linearization $\mathcal{A} - \lambda\mathcal{B}$ for non monomial basis [Amiraslani, Corless, Lancaster, 09].
  - For “clever" choice of $\mathcal{A} - \lambda\mathcal{B}$ can implement Arnoldi/rational Krylov iter. without fixing d.
    - Infinite Arnoldi [Jarlebring, Michiels, Meerbergen, 12].
    - Rational Krylov for NEP [Van Beeumen, Michiels, Meerbergen, 13].

  (See R. Van Beeumen's talk, Thur, 11:40)

Summary and Concluding Remarks

- Existence of Schur-like theorem for matrix polynomials.
- Better understanding of linearization process.
- Need to develop a backward stable algorithm for PEPs of degree larger than 2. Use of max-plus algebra.
- Rational eigenproblems with low rank matrices can be solved via linearization.
- New linearizations techniques for NEPs allowing a dynamic implementation of Arnoldi/Rational Krylov.
- Difficulties remain when the nonlinearity is difficult/impossible to approximate by a polynomial.

NLA Group in Manchester

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