Nonlinear eigenvalue problems: Analysis and numerical solution

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Mathematics for key technologies

Outline

- Lecture I:
  1. Motivation and Applications
  2. Normal and condensed forms
  3. Linearization
  4. Structure preservation
- Lecture II:
  1. Smith forms and Jordan Triples
  2. Perturbation theory
  3. Numerical methods for linear and polynomial problems
  4. Numerical methods for general nonlinear problems

Outline

Nonlinear Eigenvalue Problems

We discuss nonlinear eigenvalue problems to compute eigenvalues λ and right eigenvectors x of

$$f(\lambda, \alpha)x = 0, \ x \in \mathbb{F}^n, \ \lambda \in \mathbb{F},$$

where $\mathbb{F}$ is a field, typically $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$.

$$f : \mathbb{F} \times \mathbb{F}^p \to \mathbb{F}^\ell,$$

and α denotes a set of p parameters.
Sometimes we also want left eigenvectors $y \in \mathbb{F}^\ell$ such that

$$y^* f(\lambda, \alpha) = 0.$$

Typical functions

- Generalized linear evps $f = \lambda A_1 + A_0$.
- Quadratic evps $f = \lambda^2 A_2 + \lambda A_1 + A_0$.
- Polynomial evps $f = \sum_{i=0}^{k} \lambda^i A_i$ with coefficient matrices $A_i \in \mathbb{F}^{\ell,n}$.
- Rational evps $f = \sum_{i=-j}^{k} \lambda^i A_i$ with coefficient matrices $A_i \in \mathbb{F}^{\ell,n}$.
- General nonlinear evps f, e.g. $f = exp(\sum_{i=-j}^{k} \lambda^i A_i)$.

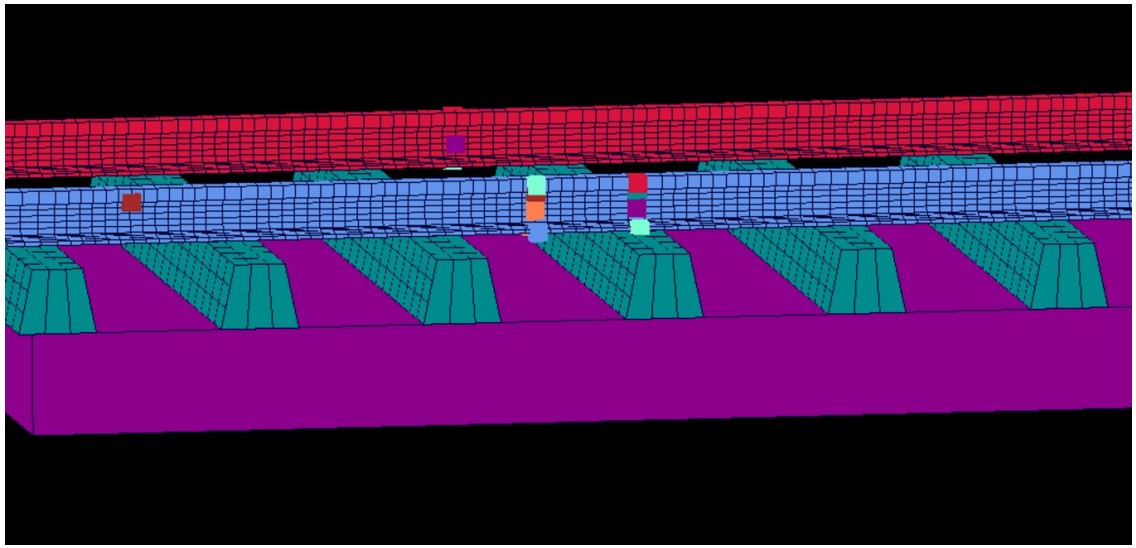
Typical questions

- Find all eigenvalues λ and associated eigenvectors x for a given parameter value α.
- Find some important eigenvalues λ and associated eigenvectors x for a given parameter α.
- Find all eigenvalues in a given subset of $\mathbb{C}$ for a given parameter α.
- Optimize eigenvalue positions over parameter set.
- ....

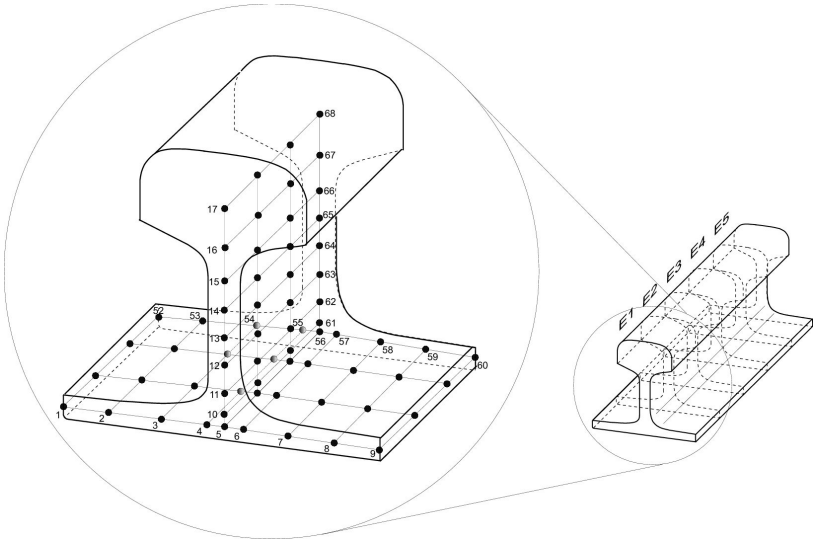
Resonances in rail tracks

Project with company SFE in Berlin 2004/2006

- Modeling of excitation of the tracks by the train.
- Discretization of rail and gravel bed with finite elements.
- Parametric eigenvalue problem for excitation frequencies.
- Optimization of parameters.
- Goal: Higher safety and reduction of noise.



Why did SFE need help?



- Even for very coarse discretization (of the track and gravel bed), commercial programs needed several hours of cpu time to solve the evp for the whole frequency range.
- Commercial packages delivered no correct digit in the evs.
- Accuracy went down when the discretization was made finer.
- Optimization of parameters not possible with current tools.

Under the assumption of an infinite rail, FEM in space leads to

$$\mathcal{M}\ddot{z} + \mathcal{D}\dot{z} + \mathcal{K}z = \mathcal{F},$$

with symmetric infinite block tridiagonal coefficient matrices (operators) $\mathcal{M}, \mathcal{D}, \mathcal{K}$, where $\mathcal{M}, z, F$ are given by

$$\begin{bmatrix} \ddots & \ddots & 0 & \dots & 0 \\ \ddots & M_{j-1,0} & M_{j,1} & 0 & \dots \\ 0 & M_{j,1}^T & M_{j,0} & M_{j+1,1} & 0 \\ \vdots & \ddots & M_{j+1,1}^T & M_{j+1,0} & M_{j+2,1} \\ 0 & \dots & 0 & \ddots & \ddots \end{bmatrix}, \begin{bmatrix} \vdots \\ z_{j-1} \\ z_j \\ z_{j+1} \\ \vdots \end{bmatrix}, \begin{bmatrix} \vdots \\ F_{j-1} \\ F_j \\ F_{j+1} \\ \vdots \end{bmatrix}.$$

Operators $\mathcal{D}, \mathcal{K}$ have the same structure as $\mathcal{M}$.
Furthermore, $M_{j,0} > 0$, $D_{j,0}$, $K_{j,0} \geq 0$.

Fourier expansion

$$F_j = \hat{F}_j e^{i\omega t},\ z_j = \hat{z}_j e^{i\omega t},$$

where ω is the excitation frequency.
Using periodicity and combining l parts into one vector

$$y_j = \begin{bmatrix} \hat{z}_j^T & \hat{z}_{j+1}^T & \cdots & \hat{z}_{j+l}^T \end{bmatrix}^T$$

gives a compley (singular) difference equation

$$A_1(\omega) y_{j+1} + A_0(\omega) y_j + A_1(\omega)^T y_{j-1} = G_j.$$

with $A_0(\omega) = A_0^T(\omega)$ block tridiagonal and $A_1(\omega)$ singular of rank smaller than $n/2$.

The associated nonlinear evp

Ansatz: $y_{j+1} = \kappa y_j$, leads to the palindromic rational eigenvalue problem

$$R(\kappa)x = (\kappa A_1(\omega) + A_0(\omega) + \frac{1}{\kappa} A_1(\omega)^T)x = 0.$$

Alternative representation as palindromic polynomial eigenvalue problem

$$P(\lambda)x = (\lambda^2 A_1(\omega) + \lambda A_0(\omega) + A_1(\omega)^T)x = 0.$$

Acoustic field computation

Industrial Project with company SFE in Berlin 2007/2011.

- Computation of acoustic field inside car.
- SFE has its own parameterized FEM model which allows geometry and topology changes. ($\rightarrow$ film)
- Problem is needed within optimization loop that changes geometry, topology, damping material, etc.
- Model reduction and reduced order models for optimization.
- Ultimate goal: Minimize noise in important regions in car interior.

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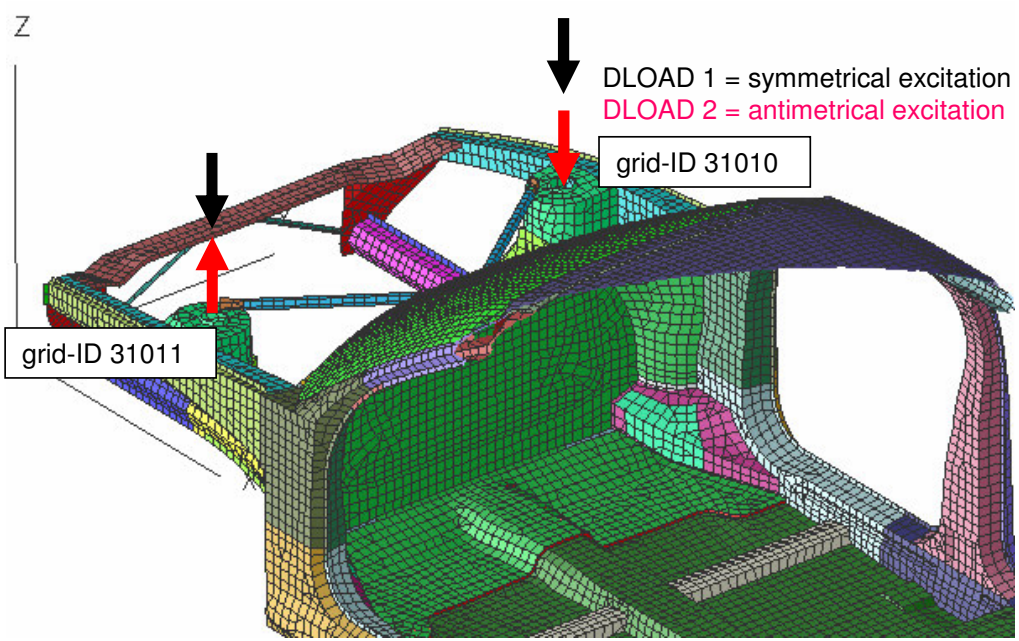
SFE AKUSMOD

FE Model: Excitation

Unit force = 1 N mm



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Tasks in the project

- Numerical methods for large scale structured parameter dependent polynomial eigenvalue problems.
- Compute eigenvalues in trapezoidal region around 0.
- Determine projectors on important spectral subspaces for model reduction.
- Model reduction for parameterized model.
- Optimization of frequencies.
- Implementation of parallel solver in SFE Concept.

Full model: summary

$$\begin{bmatrix} M_s & 0 \\ D_{sf}^T & M_f \end{bmatrix} \begin{bmatrix} \ddot{u}_d \\ \ddot{p}_d \end{bmatrix} + \begin{bmatrix} D_s & 0 \\ 0 & D_f \end{bmatrix} \begin{bmatrix} \dot{u}_d \\ \dot{p}_d \end{bmatrix} + \begin{bmatrix} K_s(\omega) & D_{sf} \\ 0 & K_f \end{bmatrix} \begin{bmatrix} u_d \\ p_d \end{bmatrix} = \begin{bmatrix} f_s \\ 0 \end{bmatrix}.$$

- M_s, M_f, K_f are real symm. pos. semidef. mass/stiffness matrices of structure and air, M_s is singular and diagonal, M_s is a factor $1000 - 10000$ larger than M_f.
- $K_s(\omega) = K_s(\omega)^T = K_1(\omega) + \imath K_2$.
- D_s, D_f are real symmetric damping matrices.
- D_{sf} is real coupling matrix between structure and air.
- Parts depend on geometry, topology and material parameters.

Eigenvalue problem

$$\left(\lambda^2 \begin{bmatrix} M_s & 0 \\ D_{sf}^T & M_f \end{bmatrix} + \lambda \begin{bmatrix} D_s & 0 \\ 0 & D_f \end{bmatrix} + \begin{bmatrix} K_s(\omega) & D_{sf} \\ 0 & K_f \end{bmatrix}\right) \begin{bmatrix} x_s \\ x_f \end{bmatrix} = 0,$$

or after scaling second block row with λ^{-1} and second block column with λ one has the complex symmetric quadratic evp

$$\left(\lambda^2 \begin{bmatrix} M_s & 0 \\ 0 & M_f \end{bmatrix} + \lambda \begin{bmatrix} D_s & D_{sf} \\ D_{sf}^T & D_f \end{bmatrix} + \begin{bmatrix} K_s(\omega) & 0 \\ 0 & K_f \end{bmatrix}\right) \begin{bmatrix} x_s \\ \lambda^{-1} x_f \end{bmatrix} = 0.$$

Outline

Linear Evps

- For linear evps $(A_0 + \lambda A_1)x = 0$ we can analyze the properties via the normal form of the pair (A_0, A_1) under equivalence transformations (PA_0Q, PA_1Q) with nonsingular matrices P, Q.
- For the special case $A_1 = I$ under similarity transformations $Q^{-1}A_0Q$ with nonsingular Q.
- For the numerical solution we want to use unitary (real orthogonal) P, Q.

Normal Forms

Problem class	Transformation	Normal form
$\lambda x + A_0 x$	$Q^{-1}AQ$, Q invertible	Jordan can. form
$\lambda A_1 x + A_0 x$,	PA_0Q, PA_1Q P, Q inv.	Kronecker can. form
$(\sum_{i=0}^{k} \lambda^i A_i)x = 0$	?	?

Theorem (Jordan canonical form (JCF))

For every $A_0 \in \mathbb{C}^{n,n}$ there exists nonsingular $Q \in \mathbb{C}^{n,n}$ such that

$$Q^{-1} A_0 \to Q = \operatorname{diag}(J_{\rho_1}, \ldots, J_{\rho_v}), \quad J_{\rho_j} = \begin{bmatrix} \lambda_j & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_j \end{bmatrix} \in \mathbb{C}^{\rho_j, \rho_j},$$

What can we learn from the JCF?

Eigenvalues, algebraic and geometric multiplicities, minimal polynomial, characteristic polynomial, left and right eigenvectors and principal vectors, invariant subspaces.

In the real case, real Jordan form.

Theorem (Kronecker canonical form (KCF))

For every pair (A_1, A_0), $A_i \in \mathbb{C}^{\ell,n}$ *there exist nonsingular* $P \in \mathbb{C}^{\ell,\ell}$, $Q \in \mathbb{C}^{n,n}$ *such that* $P(\lambda A_1 + A_0)Q =$ $\operatorname{diag}(L_{\epsilon_1}, \ldots, L_{\epsilon_p}, M_{\eta_1}, \ldots, M_{\eta_q}, J_{\rho_1}, \ldots, J_{\rho_v}, N_{\sigma_1}, \ldots, N_{\sigma_w})$, *with*

$$L_{\epsilon_j} = \lambda \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & 0 & 1 \end{bmatrix} + \begin{bmatrix} 1 & 0 & & \\ & \ddots & \ddots & \\ & & 1 & 0 \end{bmatrix}, \quad M_{\eta_j} = \lambda \begin{bmatrix} 1 & & & \\ & \ddots & & \\ 0 & & \ddots & \\ & & & 1 \\ & & & 0 \end{bmatrix} + \begin{bmatrix} 0 & & & \\ & \ddots & & \\ 1 & & \ddots & \\ & & & 0 \\ & & & 1 \end{bmatrix},$$

$$J_{\rho_j} = \lambda \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} + \begin{bmatrix} \lambda_j & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & \lambda_j \end{bmatrix}, \quad N_{\sigma_j} = \lambda \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix} + \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix}$$

Definition

A matrix pencil $\lambda A_1 + A_0,\ A_0, A_1 \in \mathbb{C}^{\ell,n}$, is called *regular* if $\ell = n$ and if

$$P(\lambda) = \det(\lambda A_1 + A_0)$$

does not vanish identically, otherwise *singular*.
The size ν_d of the largest nilpotent (N)-blocks in the KCF is called the *index* of $\lambda A_1 + A_0$.
Values $\lambda \in \mathbb{C}$ such that $\operatorname{rank}(\lambda A_1 + A_0) < \min(\ell, n)$ are called *finite eigenvalues* of $\lambda A_1 + A_0$.
The eigenvalue $\mu = 0$ of $A_1 + \mu A_0$ is called the infinite eigenvalue of $\lambda A_1 + A_0$.

Deflating subspaces

Definition

A subspace $\mathcal{L} \subset \mathbb{C}^n$ is called deflating subspace for the pencil $\lambda A_1 + A_0$ if for a matrix $X_\mathcal{L} \in \mathbb{C}^{n,r}$ with full column rank and range$X_\mathcal{L} = \mathcal{L}$ there exist matrices $Y_\mathcal{L} \in \mathbb{C}^{n,r}$, $R_\mathcal{L} \in \mathbb{C}^{r,r}$, and $S_\mathcal{L} \in \mathbb{C}^{r,r}$ such that

$$A_1 X_\mathcal{L} = Y_\mathcal{L} R_\mathcal{L}, \quad A_0 X_\mathcal{L} = Y_\mathcal{L} S_\mathcal{L}.$$

Theorem (Weierstraß canonical form (WCF))

For every regular pair (A_1, A_0), $A_i \in \mathbb{C}^{n,n}$ *there exist nonsingular* $P \in \mathbb{C}^{n,n}$, $Q \in \mathbb{C}^{n,n}$ *such that*
$P(\lambda A_1 + A_0)Q = \operatorname{diag}(J_{\rho_1}, \ldots, J_{\rho_v}, N_{\sigma_1}, \ldots, N_{\sigma_w})$, *with*

$$J_{\rho_j} = \lambda \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix} + \begin{bmatrix} \lambda_j & 1 & \\ & \ddots & \\ & & 1 \\ & & \lambda_j \end{bmatrix}, \quad N_{\sigma_j} = \lambda \begin{bmatrix} 0 & 1 & & \\ & \ddots & \ddots & \\ & & \ddots & 1 \\ & & & 0 \end{bmatrix} + \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \end{bmatrix}$$

What do learn from KCF, WCF?

- Finite eigenvalues and infinite eigenvalues.
- Algebraic and geometric multiplicities.
- Index, Kronecker indices (sizes of singular blocks).
- Regularity, non-regularity.
- Eigenvectors, principal vectors, deflating subspaces, reducing subspaces (subspaces associated with singular blocks).

Evaluation of Normal Form Approach

- The normal forms are essential for the theoretical analysis evps.
- They allow linear stability/ bifurcation analysis, the points where ranks change are a superset of the set of critical points.
- But, they cannot be used in general for the development of numerical methods
- They are typically not numerically stably computable, since the structure can be changed by arbitrary small perturbations.

Theorem (Schur form)

For every matrix $A_0 \in \mathbb{C}^{n,n}$ there exist a unitary matrix $Q \in \mathbb{C}^{n,n}$ such that

$$Q^H A_0 Q = \begin{bmatrix} \lambda_1 & * & \dots & * \\ 0 & \lambda_2 & * & * \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & \lambda_n \end{bmatrix}$$

What can we learn from Schur form ?

Eigenvalues, algebraic multiplicity, invariant subspaces.

Theorem (GUPTRI form: Demmel/Kågström 1993)

Given a matrix pair (A_1, A_0), there exist unitary matrices P, Q such that (PA_1Q, PA_0Q) are in the following generalized upper triangular form:

$$P(\lambda A_1 + A_0)Q = \begin{bmatrix} \lambda E_{11} - A_{11} & \lambda E_{12} - A_{12} & \lambda E_{13} - A_{13} & \lambda E_{14} - A_{14} \\ 0 & \lambda E_{22} - A_{22} & \lambda E_{23} - A_{23} & \lambda E_{24} - A_{24} \\ 0 & 0 & \lambda E_{33} - A_{33} & \lambda E_{34} - A_{34} \\ 0 & 0 & 0 & \lambda E_{44} - A_{44} \end{bmatrix}.$$

Here $n_2 = \ell_2, n_3 = \ell_3$, $\lambda E_{11} - A_{11}$ and $\lambda E_{44} - A_{44}$ contains all left and right singular Kronecker blocks of $\lambda A_1 + A_0$, respectively. Furthermore, $\lambda E_{22} - A_{22}$ and $\lambda E_{33} - A_{33}$ are regular and contain the regular finite and infinite structure of $\lambda A_1 + A_0$, respectively.

What can we learn form GUPTRI?

- Eigenvalues
- Algebraic multiplicity of eigenvalues.
- Left and right deflating and reducing subspaces.
- With a lot of perturbation theory also information on the length of chains.

Stably computable condensed forms

Problem class	transformation	stable cond. form
$\lambda x + A_0 x = 0$	$Q^{-1}AQ$, Q unitary	Schur form
$\lambda A_1 x + A_0 x = 0$	PA_1Q, PA_0Q, P, Q unit.	gen. Schur form
$(\sum_{i=0}^{k} \lambda^i A_i)x = 0$	?	?

Outline

Matrix polynomials

We now study polynomial evps

$$P(\lambda)\, x = (\sum_{i=0}^{k} \lambda^i A_i) x = 0,$$

where $A_i \in \mathbb{F}^{\ell,n}$.
We will extend concepts from linear to general matrix polynomials.

Definition

A matrix polynomial $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$, with $A_0, \ldots, A_k \in \mathbb{F}^{\ell,n}$, $A_k \neq 0$ is called regular if the coefficients are square matrices and if $\det P(\lambda)$ does not vanish identically for all $\lambda \in \mathbb{C}$, otherwise it is called singular.

Definition

Let $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$ with $A_0, \ldots, A_k \in \mathbb{F}^{\ell,n}$. A right (left) Jordan chain of length $r+1$ associated with a finite ev $\hat{\lambda}$ of $P(\lambda)$ is a sequence x_i (y_i), $i = 0, \ldots, r$ with $x_0, x_r \neq 0$ ($y_0, y_r \neq 0$) and

$$\begin{aligned} P(\hat{\lambda})x_0 &= 0; \\ P(\hat{\lambda})x_1 + [\tfrac{1}{1!}\tfrac{d}{d\lambda}P(\hat{\lambda})]x_0 &= 0; \\ &\vdots \\ P(\hat{\lambda})x_r + [\tfrac{1}{1!}\tfrac{d}{d\lambda}P(\hat{\lambda})]x_{r-1} + \ldots + [\tfrac{1}{r!}\tfrac{d^r}{d\lambda^r}P(\hat{\lambda})]x_0 &= 0, \end{aligned}$$

$$\begin{aligned} y_0^H P(\hat{\lambda}) &= 0; \\ y_1^H P(\hat{\lambda}) + y_0^H[\tfrac{1}{1!}\tfrac{d}{d\lambda}P(\hat{\lambda})] &= 0; \\ &\vdots \\ y_\ell^H P(\hat{\lambda}) + y_{r-1}^H[\tfrac{1}{1!}\tfrac{d}{d\lambda}P(\hat{\lambda})] + \ldots + y_0^H[\tfrac{1}{r!}\tfrac{d^r}{d\lambda^r}P(\hat{\lambda})] &= 0. \end{aligned}$$

Definition

Let $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$ with $A_0, \ldots, A_k \in \mathbb{F}^{\ell,n}$.
The reversal of $P(\lambda)$ is the polynomial

$$\operatorname{rev} P(\lambda) := \lambda^k P(1/\lambda) = \sum_{i=0}^{k} \lambda^i A_{k-i}.$$

A right (left) Kronecker chain of length $r+1$ associated with the eigenvalue infinity of $P(\lambda)$ is a right (left) Jordan chain of length $r+1$ associated with eigenvalue $\lambda = 0$ of $\operatorname{rev} P(\lambda)$.

Definition

Let $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$ with $A_0, \ldots, A_k \in \mathbb{F}^{r,n}$. A right singular Kronecker chain of length $r+1$ associated with the right singular part of $P(\lambda)$ is defined as the sequence of coefficient vectors x_i, $i = 0, \ldots, r$ in a nonzero vector polynomial $x(\lambda) = x_r\lambda^r + \ldots + x_1\lambda^1 + x_0$ of minimal degree such that $P(\lambda)x(\lambda) = 0$, considered as a polynomial equation in λ.
A left singular Kronecker chain of length $r+1$ associated with the left singular part of $P(\lambda)$ is a sequence of coefficient vectors y_i, $i = 0, \ldots, r$ in a nonzero vector polynomial $y(\lambda) = y_r\lambda^r + \ldots + y_1\lambda^1 + y_0$ of minimal degree such that $y^H(\lambda)P(\lambda) = 0$.
Here $y^H(\lambda) = y_r^H\lambda^r + \ldots + y_1^H\lambda^1 + y_0^H$.

Definition

For a matrix polynomial $P(\lambda)$, a matrix pencil $L(\lambda) = \lambda X + Y$ is called linearization of $P(\lambda)$, if there exist unimodular matrices $S(\lambda), T(\lambda)$ such that

$$S(\lambda)L(\lambda)T(\lambda) = \text{diag}(P(\lambda), I_n, \ldots, I_n).$$

If $L(\lambda)$ is a linearization for $P(\lambda)$ and $\text{rev}\ L(\lambda)$ is a linearization for $\text{rev}\ P(\lambda)$, then $L(\lambda)$ is said to be a strong linearization for $P(\lambda)$.

Properties of linearization

- Linearization preserves the algebraic and geometric multiplicities of all finite eigenvalues, but not those of infinite eigenvalues.
- Strong linearization preserves the algebraic and geometric multiplicities of all finite and infinite eigenvalues.
- The lengths of singular chains are not all invariant.

Companion linearization

The classical companion linearization for polynomial eigenvalue problems

$$P(\lambda)x = \sum_{i=0}^{k} \lambda^i A_i x$$

is to introduce new variables

$$y^T = \left[\ y_1, y_2, \ldots, y_\ell\ \right]^T = \left[\ x, \lambda x, \ldots, \lambda^{\ell-1} x\ \right]^T$$

and to turn it into a generalized linear eigenvalue problem

$$L(\lambda)y := (\lambda X + Y)y = 0$$

of size $nk \times nk$.

Difficulties with companion form

Example The even quadratic eigenvalue problem

$$(\lambda^2 M + \lambda G - K)x = 0$$

with $M = M^T, K = K^T > 0$, $G = -G^T$ has a spectrum that is symmetric with respect to both axis, but in the companion linearization

$$\begin{bmatrix} O & I \\ -K & -G \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} I & O \\ O & M \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix},$$

does not see this structure.

- Numerical methods destroy eigenvalue symmetries in finite arithmetic !
- Perturbation theory requires structured perturbation for stability near the imaginary axis.

Pros and cons of linearization

Is it a good idea to perform a linearization?

Pros

- Simpler analysis for linear eigenvalue problems.
- Not many well studied methods for matrix polynomials.
- No generalization of Jordan/Kronecker canonical form for matrix polynomials.

Cons

- The condition number (sensitivity) may increase dramatically.
- The size of the problem is increased.
- Symmetry structures may be lost.

Optimal Linearizations

Goal: Find a large class of linearizations for which:

- the linear pencil is easily constructed;
- structure preserving linearizations exist;
- the conditioning of the linear problem can be characterized and optimized;
- eigenvalues/eigenvectors of the original problem are easily read off;
- a structured perturbation analysis is possible.

Outline

Vector spaces of potential linearizations

Notation: $\Lambda := [\lambda^{k-1}, \lambda^{k-2}, \ldots, \lambda, 1]^T$, $\otimes$ - Kronecker product.

Definition Mackey[2]/Mehl/M. 2006. For a given $n \times n$ matrix polynomial $P(\lambda)$ of degree k define the sets:

$$
\begin{aligned}
\mathcal{V}_P &= \{v \otimes P(\lambda) \,:\, v \in \mathbb{F}^k\},\ v \text{ is called right ansatz vector},\\
\mathcal{W}_P &= \{w^T \otimes P(\lambda) : w \in \mathbb{F}^k\},\ w \text{ is called left ansatz vector},\\
\mathbb{L}_1(P) &= \left\{L(\lambda) = \lambda X + Y :\, X, Y \in \mathbb{F}^{kn\times kn},\ L(\lambda)\,(\Lambda \otimes I_n) \in \mathcal{V}_P\right\},\\
\mathbb{L}_2(P) &= \left\{L(\lambda) = \lambda X + Y :\, X, Y \in \mathbb{F}^{kn\times kn},\ \left(\Lambda^T \otimes I_n\right) L(\lambda) \in \mathcal{W}_P\right\}\\
\mathbb{DL}(P) &= \mathbb{L}_1(P) \cap \mathbb{L}_2(P)\,.
\end{aligned}
$$

Properties of these sets

Lemma

For any $n \times n$ matrix polynomial $P(\lambda)$ of degree k,

- $\mathbb{L}_1(P)$ *is a vector space of dimension* $k(k-1)n^2 + k$,
- $\mathbb{L}_2(P)$ *is a vector space of dimension* $k(k-1)n^2 + k$,
- $\mathbb{DL}(P)$ *is a vector space of dimension* k.

These are not all linearizations but they form a large class.

Example

Consider the cubic matrix polynomial (Antoniou and Vologiannidis 2004), $P(\lambda) = \lambda^3 A_3 + \lambda^2 A_2 + \lambda A_1 + A_0$. Then the pencil

$$L(\lambda) = \lambda \begin{bmatrix} 0 & A_3 & 0 \\ I & A_2 & 0 \\ 0 & 0 & I \end{bmatrix} + \begin{bmatrix} -I & 0 & 0 \\ 0 & A_1 & A_0 \\ 0 & -I & 0 \end{bmatrix}$$

is a linearization for P but neither in $\mathbb{L}_1(P)$ nor in $\mathbb{L}_2(P)$.

Definition (Column Shifted sum)

Let X and Y be block matrices

$$X = \begin{bmatrix} X_{11} & \cdots & X_{1k} \\ \vdots & & \vdots \\ X_{k1} & \cdots & X_{kk} \end{bmatrix}, \qquad Y = \begin{bmatrix} Y_{11} & \cdots & Y_{1k} \\ \vdots & & \vdots \\ Y_{k1} & \cdots & Y_{kk} \end{bmatrix}$$

with blocks $X_{ij}, Y_{ij} \in \mathbb{F}^{n\times n}$. Then the column shifted sum of X and Y is defined to be

$$X \boxplus\!\!\rightarrow Y := \begin{bmatrix} X_{11} & \cdots & X_{1k} & 0 \\ \vdots & & \vdots & \vdots \\ X_{k1} & \cdots & X_{kk} & 0 \end{bmatrix} + \begin{bmatrix} 0 & Y_{11} & \cdots & Y_{1k} \\ \vdots & \vdots & & \vdots \\ 0 & Y_{k1} & \cdots & Y_{kk} \end{bmatrix}.$$

The row shifted sum is defined analogously.

For the first companion form $C_1(\lambda) = \lambda X_1 + Y_1$ of $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$, the column shifted sum $X_1 \boxplus\!\!\rightarrow Y_1$ is just

$$\begin{bmatrix} A_k & 0 & \cdots & 0 \\ 0 & I_n & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & I_n \end{bmatrix} \boxplus\!\!\rightarrow \begin{bmatrix} A_{k-1} & A_{k-2} & \cdots & A_0 \\ -I_n & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & -I_n & 0 \end{bmatrix}$$

$$= \begin{bmatrix} A_k & A_{k-1} & \cdots & A_0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Lemma

Let $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$ *be an* $n \times n$ *matrix polynomial, and* $L(\lambda) = \lambda X + Y$ *a* $kn \times kn$ *pencil. Then for* $v \in \mathbb{F}^k$,

$$(\lambda X + Y)\cdot(\Lambda \otimes I_n) = v \otimes P(\lambda) \quad \Longleftrightarrow \quad X \boxplus\!\!\rightarrow Y = v \otimes [A_k \; A_{k-1} \; \cdots \; A_0],$$

and so the space $\mathbb{L}_1(P)$ *may be alternatively characterized as*

$$\mathbb{L}_1(P) = \left\{ \lambda X + Y \; : \; X \boxplus\!\!\rightarrow Y = v \otimes [A_k \; A_{k-1} \; \cdots \; A_0], \; v \in \mathbb{F}^k \right\}.$$

Analogously we can characterize $\mathbb{L}_2(P)$.

Theorem

Let $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$ be an $n \times n$ matrix polynomial, and $v \in \mathbb{F}^k$ any vector. Then the set of pencils in $\mathbb{L}_1(P)$ with right ansatz vector v consists of all $L(\lambda) = \lambda X + Y$ such that

$$X = \begin{bmatrix} v \otimes A_k & -W \end{bmatrix}$$

and

$$Y = \begin{bmatrix} W + \left(v \otimes \begin{bmatrix} A_{k-1} & \cdots & A_1 \end{bmatrix}\right) & v \otimes A_0 \end{bmatrix}.$$

with $W \in \mathbb{F}^{kn \times (k-1)n}$ chosen arbitrarily.

Corollary

$\mathbb{L}_2(P) = \left[\mathbb{L}_1(P^T)\right]^T$.

Procedure for linearization condition for $\mathbb{L}_1(P)$.

1) Suppose $P(\lambda)$ is regular and $L(\lambda) = \lambda X + Y \in \mathbb{L}_1(P)$ has $0 \neq v \in \mathbb{F}^k$, i.e., $L(\lambda) \cdot (\Lambda \otimes I_n) = v \otimes P(\lambda)$.
2) Select any nonsingular matrix M such that $Mv = \alpha e_1$.
3) Form $\widetilde{L}(\lambda) := (M \otimes I_n)L(\lambda)$, which must be of the form

$$\widetilde{L}(\lambda) = \lambda\widetilde{X} + \widetilde{Y} = \lambda \left[\begin{array}{c|c} \widetilde{X}_{11} & \widetilde{X}_{12} \\ \hline 0 & -Z \end{array}\right] + \left[\begin{array}{c|c} \widetilde{Y}_{11} & \widetilde{Y}_{12} \\ \hline Z & 0 \end{array}\right],$$

   where $\widetilde{X}_{11}$ and $\widetilde{Y}_{12}$ are $n \times n$.
4) Check $\boxed{\det Z \neq 0}$, the linearization condition for $L(\lambda)$.

This procedure can be implemented as a numerical algorithm: choose M to be unitary, then use a rank revealing factorization to check if Z is nonsingular.

Consider a general regular $P(\lambda) = \lambda^2 A + \lambda B + C$, and

$$L(\lambda) = \lambda \begin{bmatrix} A & B+C \\ A & 2B-A \end{bmatrix} + \begin{bmatrix} -C & C \\ A-B & C \end{bmatrix}.$$

Since

$$\begin{bmatrix} A & B+C \\ A & 2B-A \end{bmatrix} \boxplus\!\!\rightarrow \begin{bmatrix} -C & C \\ A-B & C \end{bmatrix} = \begin{bmatrix} A & B & C \\ A & B & C \end{bmatrix},$$

we have $L(\lambda) \in \mathbb{L}_1(P)$ with right ansatz vector $v = \begin{bmatrix} 1 & 1 \end{bmatrix}^T$. Subtracting the first entry from the second reduces v to e_1, and the corresponding block-row-operation on Y yields

$$\widetilde{Y} = \begin{bmatrix} -C & C \\ A-B+C & 0 \end{bmatrix}.$$

Hence $Z = A - B + C$, and we have a linearization iff $\det(A - B + C) = \det P(-1) \neq 0$, i.e., $\lambda = -1$ is *not* an eigenvalue of P.

Consider the general regular cubic polynomial $P(\lambda) = \lambda^3 A + \lambda^2 B + \lambda C + D$ and the pencil

$$\lambda X + Y = \lambda \begin{bmatrix} A & 0 & 2C \\ -2A & -B-C & D-4C \\ 0 & A & -I \end{bmatrix} + \begin{bmatrix} B & -C & D \\ C-B & 2C-D & -2D \\ -A & I & 0 \end{bmatrix}$$

in $\mathbb{L}_1(P)$. Since $X \boxplus\!\!\rightarrow Y = \begin{bmatrix} 1 & -2 & 0 \end{bmatrix}^T \otimes \begin{bmatrix} A & B & C & D \end{bmatrix}$, we have $v = \begin{bmatrix} 1 & -2 & 0 \end{bmatrix}^T$. Adding twice the first block-row of Y to the second block-row of Y gives

$$Z = \begin{bmatrix} B+C & -D \\ -A & I \end{bmatrix},$$

and hence the condition $\det Z = \det(B + C - DA) \neq 0$.

Eigenvector Recovery Property

Theorem

Let $P(\lambda)$ be an $n \times n$ matrix polynomial of degree k, and let $L(\lambda)$ be any pencil in $\mathbb{L}_1(P)$ with ansatz vector $v \neq 0$.

Then $x \in \mathbb{C}^n$ is a right eigenvector for $P(\lambda)$ with finite eigenvalue $\lambda \in \mathbb{C}$ if and only if $\Lambda \otimes x$ is a right eigenvector for $L(\lambda)$ with eigenvalue λ.

If in addition P is regular, i.e. $\det P(\lambda) \not\equiv 0$, and $L \in \mathbb{L}_1(P)$ is a linearization then every eigenvector of L with finite eigenvalue λ is of the form $\Lambda \otimes x$ for some eigenvector x of P.

A similar result holds for the space $\mathbb{L}_2(P)$ and also for eigenvalues $0, \infty$.

Strong Linearization Property

Theorem

Let $P(\lambda)$ be a regular matrix polynomial and $L(\lambda) \in \mathbb{L}_1(P)$ (or $L(\lambda) \in \mathbb{L}_2(P)$). Then the following statements are equivalent.

(i) *$L(\lambda)$ is a linearization for $P(\lambda)$.*

(ii) *$L(\lambda)$ is a regular pencil.*

(iii) *$L(\lambda)$ is a strong linearization for $P(\lambda)$.*

The first and second companion forms

$$C_1(\lambda) := \lambda \begin{bmatrix} A_k & 0 & \cdots & 0 \\ 0 & I_n & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & I_n \end{bmatrix} + \begin{bmatrix} A_{k-1} & A_{k-2} & \cdots & A_0 \\ -I_n & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & -I_n & 0 \end{bmatrix}$$

$$C_2(\lambda) := \lambda \begin{bmatrix} A_k & 0 & \cdots & 0 \\ 0 & I_n & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & I_n \end{bmatrix} + \begin{bmatrix} A_{k-1} & -I_n & \cdots & 0 \\ A_{k-2} & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & -I_n \\ A_0 & 0 & \cdots & 0 \end{bmatrix}.$$

are strong linearizations in $\mathbb{L}_1(P)$, $\mathbb{L}_2(P)$, respectively.

Characterization of $\mathbb{DL}(P)$

Lemma

Consider an $n \times n$ matrix polynomial $P(\lambda)$ of degree k. Then, for $v = (v_1, \ldots, v_k)^T$ and $w = (w_1, \ldots, w_k)^T$ in $\mathbb{F}^k$, the associated pencil satisfies $L(\lambda) = \lambda X + Y \in \mathbb{DL}(P)$ if and only if $v = w$.

Once an ansatz vector v has been chosen, a pencil from $\mathbb{DL}(P)$ is uniquely determined.

Are the classes large enough?

Theorem

For any regular $n \times n$ matrix polynomial $P(\lambda)$ of degree k, almost every pencil in $\mathbb{L}_1(P)$ ($\mathbb{L}_2(P)$) is a linearization for $P(\lambda)$.

For any regular matrix polynomial $P(\lambda)$, pencils in $\mathbb{DL}(P)$ are linearizations of $P(\lambda)$ for almost all $v \in \mathbb{F}^k$.

'Almost every' means for all but a closed, nowhere dense set of measure zero.

Linearization property for $\mathbb{DL}(P)$

Theorem

Consider an $n \times n$ matrix polynomial $P(\lambda)$ of degree k. Then for given ansatz vector $v = w = [v_1, \ldots, v_k]^T$ the associated linear pencil in $\mathbb{DL}(P)$ is a linearization if and only if no root of the v-polynomial

$$p(v; x) := v_1 x^{k-1} + \ldots + v_{k-1} x + v_k$$

is an eigenvalue of P.

Consider $P(\lambda) = \lambda^3 A + \lambda^2 B + \lambda C + D$ and

$$L(\lambda) = \lambda \begin{bmatrix} A & 0 & -A \\ 0 & -A-C & -B-D \\ -A & -B-D & -C \end{bmatrix} + \begin{bmatrix} B & A+C & D \\ A+C & B+D & 0 \\ D & 0 & -D \end{bmatrix}$$

in $\mathbb{DL}(P)$ with ansatz vector $v = \begin{bmatrix} 1 & 0 & -1 \end{bmatrix}^T$,

$$p(v; x) = x^2 - 1.$$

Using the check one easily finds that

$$\det \begin{bmatrix} A+C & B+D \\ B+D & A+C \end{bmatrix} \neq 0$$

is the linearization condition for $L(\lambda)$.
This is equivalent to saying that neither -1 nor $+1$ is an eigenvalue of the matrix polynomial $P(\lambda)$.

Outline

Polynomial evps with structure

$$P(\lambda)\, x = 0,$$

where

- $P(\lambda)$ is polynomial matrix valued function;
- x is a real or complex eigenvector;
- λ is a real or complex eigenvalue;
- and $P(\lambda)$ has some further structure.

Which structures?

Definition

A nonlinear matrix polynomial $P(\lambda)$ of degree k is called

- **T-even (H-even)** if $P(\lambda) = P^T(-\lambda)$ $(P(\lambda) = P^H(-\lambda))$;
- **T-palindromic (H-palindromic)** if $P(\lambda) = P^T(\lambda^{-1})\lambda^k$ $(P(\lambda) = P^H(\lambda^{-1})\lambda^k$.
- **T-symmetric (Hermitian)** if $P(\lambda) = P^T(\lambda)$ $(P(\lambda)^H = P(\lambda))$;

Examples

- A T-even quadratic problem has the form $\lambda^2 M + \lambda G + K$ with $M = M^T, K = K^T, G = -G^T$.
- A H-palindromic cubic problem has the form $\lambda^3 A_3 + \lambda^2 A^2 + \lambda A_1 + A_0$ where $A_3 = A_0^H, A_2 = A_1^H$.
- A quadratic symmetric problem has the form $\lambda^2 M + \lambda D + K$, with $M = M^T, K = K^T, D = D^T$.

Properties of even matrix functions

Lemma

Consider a T-even eigenvalue problem $P(\lambda)x = 0$. Then $P(\lambda)x = 0$ if and only if $x^T P(-\lambda) = 0$, i.e., the eigenvalues occur in pairs λ, $-\lambda$, or quadruples λ, $-\lambda$, $\bar{\lambda}$, $-\bar{\lambda}$ in the real case.

Consider a H-even eigenvalue problem $P(\lambda)x = 0$. Then $P(\lambda)x = 0$ if and only if $x^H P(-\bar{\lambda}) = 0$, i.e., the eigenvalues occur in pairs λ, $-\bar{\lambda}$

Even matrix functions have Hamiltonian spectrum, they generalize Hamiltonian problems $\lambda I + \mathcal{H}$, where $\mathcal{H}$ is Hamiltonian.

Properties of palindromic matrix functions

Lemma

Consider a T-palindromic eigenvalue problem $P(\lambda)x = 0$. Then $P(\lambda)x = 0$ if and only if $x^T P(1/\lambda) = 0$, i.e., the eigenvalues occur in pairs λ, $1/\lambda$ or quadruples λ, $1/\lambda$, $\bar{\lambda}$, $1/\bar{\lambda}$ in the real case.

Consider a H-palindromic eigenvalue problem $P(\lambda)x = 0$. Then $P(\lambda)x = 0$ if and only if $x^T P(1/\bar{\lambda}) = 0$, i.e., the eigenvalues occur in pairs λ, $1/\bar{\lambda}$.

Palindromic matrix functions have symplectic spectrum, they generalize symplectic problems $\lambda I + \mathcal{S}$, where $\mathcal{S}$ is a symplectic matrix.

Properties of symmetric matrix functions

In general symmetric/Hermition matrix functions have no special symmetries in the spectrum. Left and right eigenvectors to an eigenvalue, however, are the same.
In some special cases (definite, hyperbolic) it can be shown that all eigenvalues are real or purely imaginary.
Example Consider the quadratic problem $\lambda^2 M + K$ with M, K real symmetric, M positive definite, K positive semidefinite. Then the eigenvalues are the square roots of the negative eigenvalues of $-L^{-1}KL^{-T}$ and thus purely imaginary.

Even Matrix Polynomials

- Singularities (cracks) in anisotropic materials as functions of material or geometry parameters
- Optimal control of differential equations
- Gyroscopic systems
- Optimal Waveguide Design,
- H_∞ control

Palindromic Matrix Polynomials

- Excitation of rail tracks by high speed trains
- Periodic surface acoustic wave filters
- Control of (high order) difference equations
- Computation of the Crawford number

Symmetric/Hermitian Matrix Polynomials

- Mass, spring, damper systems, dynamic simulation of structures.
- Acoustic field problem.
- Quantum dot simulation.
- ...

Outline

Lemma

Consider an $n \times n$ even matrix polynomial $P(\lambda)$ of degree k.

For an ansatz vector $v = (v_1, \ldots, v_k)^T \in \mathbb{F}^k$ the linearization $L(\lambda) = \lambda X + Y \in \mathbb{DL}(P)$ is even, i.e. $X = X^T$ and $Y = -Y^T$, if and only if $p(v; x)$ is even.

Consider an $n \times n$ palindromic matrix polynomial $P(\lambda)$ of degree k.

Then, for a vector $v = (v_1, \ldots, v_k)^T \in \mathbb{F}^k$ the linearization $L(\lambda) = \lambda X + Y \in \mathbb{DL}(P)$ is (the permutation of) a palindromic, if and only if $p(v; x)$ is palindromic.

Example

For the palindromic polynomial

$$P(\lambda)y = (\lambda^2 A_1^T + \lambda A_0 + A_1)y = 0,\ A_0 = A_0^T$$

a palindromic vector $v = [\alpha, \alpha]^T$, $\alpha \neq 0$ leads to a palindromic pencil

$$(\kappa Z + Z^T)z = 0,\ Z = \begin{bmatrix} A_1^T & A_0 - A_1 \\ A_1^T & A_1^T \end{bmatrix}.$$

This is a linearization if and only if -1 is not an eigenvalue of $P(\lambda)$.

Symmetric linearizations

For symmetric P, a simple argument shows that every pencil in $\mathbb{DL}(P)$ is also symmetric:
$L \in \mathbb{DL}(P)$ with ansatz vector v implies that L^T is also in $\mathbb{DL}(P)$ with the *same* ansatz vector v, and then $L = L^T$ follows from the uniqueness.

Deflation of 'bad eigenvalues'

To have structure preserving linearizations we need to deflate bad eigenvalues and singular blocks first.

- Open Question: Can we linearize first and then deflate in the linear problem?
- If so, then we need structure preserving procedures for even (palindromic) pencils.
- Do we have structured Kronecker forms?

Outline

Structured Kronecker form

To preserve the even, palindromic, symmetric structure, we use congruence transformations

$$\begin{aligned}
\lambda\tilde{N}+\tilde{M} &= \lambda U^T N U + U^T M U,\\
\lambda\tilde{A}^T+\tilde{A} &= \lambda U^T A^T U + U^T A U,\\
\lambda\tilde{M}+\tilde{K} &= \lambda U^T M U + U^T K U,\\
\lambda\tilde{N}+\tilde{M} &= \lambda U^H N U + U^H M U,\\
\lambda\tilde{A}^T+\tilde{A} &= \lambda U^T A^T U + U^T A U,\\
\lambda\tilde{M}+\tilde{K} &= \lambda U^H M U + U^H K U,
\end{aligned}$$

with nonsingular (orthogonal, unitary) U.

What are the structured canonical condensed forms under these transformations?

Theorem (Thompson 91)

If $N, M \in \mathbb{R}^{n,n}$ with $N = -N^T, M = M^T$, then there exists a nonsingular matrix $X \in \mathbb{C}^{n,n}$ such that

$$X^T(\lambda N + M)X = \operatorname{diag}(\mathcal{B}_{\mathcal{S}}, \mathcal{B}_{\mathcal{I}}, \mathcal{B}_{\mathcal{Z}}, \mathcal{B}_{\mathcal{F}}),$$

$$\begin{aligned}
\mathcal{B}_{\mathcal{S}} &= \operatorname{diag}(\mathcal{O}_\eta, \mathcal{S}_{\xi_1}, \ldots, \mathcal{S}_{\xi_k}), \\
\mathcal{B}_{\mathcal{I}} &= \operatorname{diag}\left(\mathcal{I}_{2\epsilon_1+1}, \ldots, \mathcal{I}_{2\epsilon_l+1}, \mathcal{I}_{2\delta_1}, \ldots, \mathcal{I}_{2\delta_m}\right), \\
\mathcal{B}_{\mathcal{Z}} &= \operatorname{diag}\left(\mathcal{Z}_{2\sigma_1+1}, \ldots, \mathcal{Z}_{2\sigma_r+1}, \mathcal{Z}_{2\rho_1}, \ldots, \mathcal{Z}_{2\rho_s}\right), \\
\mathcal{B}_{\mathcal{F}} &= \operatorname{diag}(\mathcal{R}_{\phi_1}, \ldots, \mathcal{R}_{\phi_t}, \mathcal{C}_{\psi_1}, \ldots, \mathcal{C}_{\psi_u})
\end{aligned}$$

This structured Kronecker canonical form is unique up to permutation of the blocks.

1. $\mathcal{O}_\eta = \lambda 0_\eta + 0_\eta$;
2. Each $\mathcal{S}_{\xi_j}$ is a $(2\xi_j + 1) \times (2\xi_j + 1)$ block that combines a right singular block and a left singular block, both of minimal index ξ_j. It has the form

$$\lambda \left[\begin{array}{ccc|ccc} & & -1 & & & 1 \; 0 \\ & \iddots & 0 & & \iddots & \iddots \\ -1 & \iddots & & 1 & 0 & \\ \hline 0 & & & & & \end{array}\right] + \left[\begin{array}{ccc|ccc} & & 0 & & & 0 \; 1 \\ & \iddots & 1 & & \iddots & \iddots \\ 0 & \iddots & & 0 & 1 & \\ \hline 1 & & & & & \end{array}\right];$$

3. Each $\mathcal{I}_{2\epsilon_j+1}$ is a $(2\epsilon_j+1)\times(2\epsilon_j+1)$ block that contains a single block corresponding to the eigenvalue ∞ with index $2\epsilon_j+1$. It has the form

$$\lambda\left[\begin{array}{ccc|ccc} & & & & & 1 & 0 \\ & & & & \iddots & \iddots & \\ & & & 1 & 0 & & \\ \hline & & -1 & 0 & & & \\ & \iddots & 0 & & & & \\ -1 & \iddots & & & & & \\ 0 & & & & & & \end{array}\right]+\left[\begin{array}{ccc|ccc} & & & & & 0 & 1 \\ & & & & \iddots & \iddots & \\ & & & 0 & 1 & & \\ \hline & & 0 & s & & & \\ & \iddots & 1 & & & & \\ 0 & \iddots & & & & & \\ 1 & & & & & & \end{array}\right],$$

where $s\in\{1,-1\}$ is the sign-index or sign-characteristic of the block;

4. Each $\mathcal{I}_{2\delta_j}$ is a $4\delta_j \times 4\delta_j$ block that combines two $2\delta_j \times 2\delta_j$ infinite eigenvalue blocks of index δ_j. It has the form

$$\lambda \left[\begin{array}{cc|cc} & & 1 & 0 \\ & & \iddots & \iddots \\ & & 1 & \iddots \\ & & 0 & \\ \hline & -1 & 0 & \\ \iddots & \iddots & & \\ -1 & \iddots & & \\ 0 & & & \end{array}\right] + \left[\begin{array}{cc|cc} & & & 1 \\ & & & \iddots \\ & & 1 & \\ \hline & 1 & & \\ \iddots & & & \\ 1 & & & \end{array}\right];$$

5. Each $\mathcal{Z}_{2\sigma_j+1}$ is a $(4\sigma_j+2)\times(4\sigma_j+2)$ block that combines two $(2\sigma_j+1)\times(2\sigma_j+1)$ Jordan blocks corresponding to the eigenvalue 0. It has the form

$$\lambda\begin{bmatrix} & & & & 1\\ & & & \iddots & \\ & & 1 & & \\ & -1 & & & \\ \iddots & & & & \\ -1 & & & & \end{bmatrix}+\begin{bmatrix} & & & & 1 & 0\\ & & & \iddots & \iddots & \\ & & 1 & \iddots & & \\ & 0 & & & & \\ & & 1 & 0 & & \\ \iddots & & \iddots & & & \\ 1 & \iddots & & & & \\ 0 & & & & & \end{bmatrix};$$

6. Each $\mathcal{Z}_{2\rho_j}$ is a $2\rho_j \times 2\rho_j$ block that contains a single Jordan block corresponding to the eigenvalue 0. It has the form

$$\lambda \left[\begin{array}{cc|cc} & & & 1 \\ & & \iddots & \\ & & 1 & \\ \hline & -1 & & \\ \iddots & & & \\ -1 & & & \end{array}\right] + \left[\begin{array}{cc|cc} & & 1 & 0 \\ & & \iddots & \iddots \\ & & 1 & \iddots \\ \hline & & s & 0 \\ & 1 & 0 & \\ \iddots & \iddots & & \\ 1 & \iddots & & \\ 0 & & & \end{array}\right],$$

where $s \in \{1, -1\}$ is the sign characteristic of this block;

7. Each $\mathcal{R}_{\phi_j}$ is a $2\phi_j \times 2\phi_j$ block that combines two $\phi_j \times \phi_j$ Jordan blocks corresponding to nonzero real eigenvalues a_j and $-a_j$. It has the form

$$\lambda \left[\begin{array}{cc|cc} & & & 1 \\ & & & \iddots \\ & & 1 & \\ & -1 & & \\ \iddots & & & \\ -1 & & & \end{array}\right] + \left[\begin{array}{cc|cc} & & & 1 \quad a_j \\ & & \iddots & \iddots \\ & & 1 & a_j \\ & 1 \quad a_j & & \\ \iddots & \iddots & & \\ 1 & \iddots & & \\ a_j & & & \end{array}\right].$$

8 a. Either $\mathcal{C}_{\psi_j}$ is a $2\psi_j \times 2\psi_j$ block combining two $\psi_j \times \psi_j$ Jordan blocks with purely imaginary eigenvalues $ib_j, -ib_j$ ($b_j > 0$). It has the form

$$\lambda \begin{bmatrix} & & & 1 \\ & & \iddots & \\ & 1 & & \\ -1 & & & \\ & \iddots & & \\ -1 & & & \end{bmatrix} + s \begin{bmatrix} & & 1 & b_j & & & \\ & \iddots & \iddots & & & & \\ 1 & \iddots & & & & & \\ b_j & & & & & & \\ & & & & & 1 & b_j \\ & & & & \iddots & \iddots & \\ & & & & 1 & \iddots & \\ & & & & b_j & & \end{bmatrix},$$

where $s \in \{1, -1\}$ is the sign characteristic.

8 b. or $\mathcal{C}_{\psi_j}$ is a $4\psi_j \times 4\psi_j$ block combining $\psi_j \times \psi_j$ Jordan blocks for each of the complex eigenvalues $a_j + ib_j, a_j - ib_j, -a_j + ib_j, -a_j - ib_j$ (with $a_j \neq 0$ and $b_j \neq 0$). In this case it has form

$$\lambda \begin{bmatrix} & & & \Omega \\ & & \iddots & \\ & \Omega & & \\ -\Omega & & & \end{bmatrix} + \begin{bmatrix} & & & \Omega & \Lambda_j \\ & & \iddots & \iddots & \\ & \Omega & \Lambda_j & & \\ & \iddots & \iddots & & \\ \Omega & \iddots & & & \\ \Lambda_j & & & & \end{bmatrix}$$

with $\Omega = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ and $\Lambda_j = \begin{bmatrix} -b_j & a_j \\ a_j & b_j \end{bmatrix}$.

Structured KCF for palindromic pencils

Theorem (Horn/Sergejchuk 06, Schröder 06)

If $A \in \mathbb{R}^{n,n}$, then there exists a nonsingular matrix $X \in \mathbb{R}^{n,n}$ such that

$$\lambda X^T A^T X + X^T A X = \operatorname{diag}(\lambda A_1 + A_1^T, \ldots, \lambda A_\ell^T + A_\ell)$$

is in structured Kronecker form.
This structured Kronecker canonical form is unique up to permutation of blocks, i.e., the kind, size and number of the blocks as well as the sign characteristics are characteristic of the pencil $\lambda A^T + A$.

$$S_p = \left[\begin{array}{cc|cc} & & & 0 \\ & 0_{p+1} & & \iddots \; 1 \\ & & 0 & \iddots \\ & & 1 & \\ \hline & 1 \quad 0 & & \\ & \iddots \quad \iddots & & 0_p \\ 1 & \quad 0 & & \end{array}\right] \in \mathbb{R}^{2p+1,2p+1}, p \in \mathbb{N}_0;$$

$$L_{1,p}(\lambda) = \left[\begin{array}{cc|cc} & & & \lambda \\ & 0_p & & \iddots \; 1 \\ & & \iddots & \iddots \\ & & \lambda \quad 1 & \\ \hline & & 1 & \\ & \iddots & & \\ & \iddots & & 0_p \\ 1 & & & \end{array}\right] \in \mathbb{R}^{2p,2p},$$

where $p \in \mathbb{N}, \lambda \in \mathbb{R}, |\lambda| < 1;$

$$L_{2,p}(\alpha,\beta) = \left[\begin{array}{c|c} 0_{2p} & \begin{matrix} & & \Lambda \\ & \iddots & I_2 \\ \Lambda & \iddots & \\ I_2 & & \end{matrix} \\ \hline \begin{matrix} & & I_2 \\ & \iddots & \\ I_2 & & \end{matrix} & 0_{2p} \end{array}\right] \in \mathbb{R}^{4p,4p},$$

where $p \in \mathbb{N}, \Lambda = \begin{bmatrix} \alpha & -\beta \\ \beta & \alpha \end{bmatrix}, \alpha, \beta \in \mathbb{R} \setminus \{0\}, \beta < 0, |\alpha + i\beta| < 1;$

$$\sigma U_{1,p} = \sigma \left[\begin{array}{c|c|c} 0_{\lfloor \frac{p}{2} \rfloor} & & \begin{matrix} & & 1 \\ & \iddots & 1 \\ 1 & \iddots & \end{matrix} \\ \hline & 1 \; 1 & \\ \hline \begin{matrix} & & 1 \\ & \iddots & \\ 1 & & \end{matrix} & & 0_{\lfloor \frac{p}{2} \rfloor} \end{array}\right] \in \mathbb{R}^{p,p},$$ where $p \in \mathbb{N}$ is odd,

$\sigma \in \{1, -1\};$

$$U_{2,p} = L_p(1) = \left[\begin{array}{c|c} 0_p & \begin{array}{cc} & 1 \\ \iddots & 1 \\ 1 & 1 \end{array} \\ \hline \begin{array}{cc} 1 & \\ \iddots & \\ & \end{array} & 0_p \end{array}\right] \in \mathbb{R}^{2p,2p},$$

where $p \in \mathbb{N}$ is even;

$$U_{3,p} = L_p(-1) = \left[\begin{array}{c|c} 0_p & \begin{array}{cc} & -1 \\ \iddots & 1 \\ -1 & 1 \end{array} \\ \hline \begin{array}{cc} 1 & \\ \iddots & \\ & \end{array} & 0_p \end{array}\right] \in \mathbb{R}^{2p,2p},$$ where $p \in \mathbb{N}$ is odd;

$$\sigma U_{4,p} = \sigma \left[\begin{array}{cc|cc} & & & -1 \\ & 0_{\frac{p}{2}} & & 1 \\ & & -1 & 1 \\ \hline & & 1 & 1 \\ & \iddots & & \\ \iddots & & & \\ 1 & & & \end{array}\right] \in \mathbb{R}^{p,p},$$

where $p \in \mathbb{N}$ is even, $\sigma \in \{1, -1\}$;

$$\sigma U_{5,p}(\alpha,\beta) = \sigma \left[\begin{array}{cc|c|cc} & & & & \Lambda \\ & 0_{2\lfloor\frac{p}{2}\rfloor} & & & \ddots \\ & & & \Lambda & \ddots \\ \hline & & \Lambda^{\frac{1}{2}} & I_2 & \\ \hline & I_2 & & & \\ & \ddots & & 0_{2\lfloor\frac{p}{2}\rfloor} & \\ I_2 & & & & \end{array}\right] \in \mathbb{R}^{2p,2p},$$

where $p \in \mathbb{N}$ is odd, $|\alpha + i\beta| = 1, \beta < 0, \Lambda = \begin{bmatrix} \alpha & -\beta \\ \beta & \alpha \end{bmatrix}$,

$\Lambda^{\frac{1}{2}}$ is defined as rotation matrix with rotation angle $\frac{\phi}{2} \in (0, \pi)$, where $\phi = \arctan(\frac{\beta}{\alpha})$ is the rotation angle of the rotation matrix Λ, $\sigma \in \{1, -1\}$;

$$\sigma U_{6,p}(\alpha,\beta) = \sigma \left[\begin{array}{cc|cc} & & & \Lambda \\ & 0_{2\frac{p}{2}} & & \iddots \; I_2 \\ & & \iddots & \iddots \\ \hline & & \Lambda \; I_2 & \\ & I_2 & I_2 & \\ & \iddots & & \\ I_2 & & & \end{array}\right] \in \mathbb{R}^{2p,2p},$$

where $p \in \mathbb{N}$ is even,

$$|\alpha + i\beta| = 1, \beta < 0, \Lambda = \begin{bmatrix} \alpha & -\beta \\ \beta & \alpha \end{bmatrix}, \sigma \in \{1, -1\}.$$

Other structured KCF

- Analogous results for symmetric pencils.
- Analogous results exist for complex even pencils.
- Analogous results exist for complex palindromic pencils.
- Hermitian pencils and complex T-symmetric pencils can be treated like complex even pencils (Set $\lambda = i\mu$).

Consequences

- Even, palindromic, symmetric KCF for pencils exist.
- But the transformation matrix X may be arbitrarily ill-conditioned.
- The even, palindromic, symmetric KCF cannot be computed well with finite precision algorithms.
- The information given in the even, palindromic, symmetric KCF is essential for the understanding of the computational problems.
- We need alternatives, from which we can derive the information, that allows the deflation of singular blocks and blocks associated with $0, \infty$ (1 and -1).

Outline

Why not just $\lambda QNU + QMU$?

Example Consider a 3×3 even pencil with matrices

$$N = Q \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} Q^T, \qquad M = Q \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} Q^T,$$

where Q is a random real orthogonal matrix. The pencil is congruent to

$$\lambda \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

For different randomly generated orthogonal matrices Q the QZ algorithm in MATLAB produced all variations of eigenvalues that are possible in a general 3×3 pencil.

Structured staircase form for even pencils

Theorem (Byers/M./Xu 07)

For $\lambda N + M$ with $N = -N^T, M = M^T \in \mathbb{R}^{n,n}$, there exists a real orthogonal matrix $U \in \mathbb{R}^{n,n}$, such that

$$U^T N U = \left[\begin{array}{ccccc|c|ccc|c} N_{11} & \cdots & \cdots & N_{1,m} & N_{1,m+1} & N_{1,m+2} & \cdots & N_{1,2m} & 0 & n_1 \\ \vdots & \ddots & & \vdots & \vdots & \vdots & \iddots & \iddots & & \vdots \\ \vdots & & \ddots & \vdots & \vdots & N_{m-1,m+2} & \iddots & & & \vdots \\ -N_{1,m}^T & \cdots & \cdots & N_{m,m} & N_{m,m+1} & 0 & & & & n_m \\ \hline -N_{1,m+1}^T & \cdots & \cdots & -N_{m,m+1}^T & N_{m+1,m+1} & & & & & l \\ \hline -N_{1,m+2}^T & \cdots & -N_{m-1,m+2}^T & 0 & & & & & & q_m \\ \vdots & \iddots & \iddots & & & & & & & \vdots \\ -N_{1,2m}^T & \iddots & & & & & & & & q_2 \\ 0 & & & & & & & & & q_1 \end{array}\right]$$

$$U^T M U = \left[\begin{array}{ccc|c|cc|c} M_{11} & \cdots & M_{1,m} & M_{1,m+1} & M_{1,m+2} & \cdots & M_{1,2m+1} \\ \vdots & \ddots & \vdots & \vdots & \vdots & \iddots & \\ M_{1,m}^T & \cdots & M_{m,m} & M_{m,m+1} & M_{m,m+2} & & \\ \hline M_{1,m+1}^T & \cdots & M_{m,m+1}^T & M_{m+1,m+1} & & & \\ \hline M_{1,m+2}^T & \cdots & M_{m,m+2}^T & & & & \\ \vdots & \iddots & & & & & \\ M_{1,2m+1}^T & & & & & & \end{array}\right] \begin{array}{c} n_1 \\ \vdots \\ n_m \\ \hline l \\ \hline q_m \\ \vdots \\ q_1 \end{array},$$

where $q_1 \geq n_1 \geq q_2 \geq n_2 \geq \ldots \geq q_m \geq n_m$,

$$\begin{aligned} N_{j,2m+1-j} &\in \mathbb{R}^{n_j,q_{j+1}}, \quad 1 \leq j \leq m-1, \\ N_{m+1,m+1} &= \begin{bmatrix} \Delta & 0 \\ 0 & 0 \end{bmatrix}, \quad \Delta = -\Delta^T \in \mathbb{R}^{2p,2p}, \\ M_{j,2m+2-j} &= \begin{bmatrix} \Gamma_j & 0 \end{bmatrix} \in \mathbb{R}^{n_j,q_j}, \quad \Gamma_j \in \mathbb{R}^{n_j,n_j}, \quad 1 \leq j \leq m, \\ M_{m+1,m+1} &= \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12}^T & \Sigma_{22} \end{bmatrix}, \quad \Sigma_{11} = \Sigma_{11}^T \in \mathbb{R}^{2p,2p}, \quad \Sigma_{22} = \Sigma_{22}^T \in \mathbb{R}^{l-2p,l-2p}, \end{aligned}$$

and the blocks Σ_{22} and Δ and Γ_j, $j = 1, \ldots, m$ are nonsingular.

- The middle block

$$\lambda N_{m+1,m+1} + M_{m+1,m+1} = \lambda \begin{bmatrix} \Delta & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} \Sigma_{11} & \Sigma_{12} \\ \Sigma_{12}^T & \Sigma_{22} \end{bmatrix},$$

  contains all the blocks associated with finite eigenvalues and 1×1 blocks associated with the eigenvalue ∞.
- The finite spectrum of is obtained from the even pencil $\lambda\Delta + \Sigma = \lambda\Delta + (\Sigma_{11} - \Sigma_{12}\Sigma_{22}^{-1}\Sigma_{12}^T)$ with Δ invertible.
- The matrix Δ has a skew-Cholesky factorization $\Delta = LJL^T$, with $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$,
- The spectral information can be obtained from the Hamiltonian matrix $\mathcal{H} = JL^{-1}\Sigma L^{-T}$.

Consequences, other cases

- Similar staircase forms for palindromic, symmetric pencils.
- All the information about the invariants (Kronecker indices) can be read off. Byers/M./Xu 07.
- Bad eigenvalues can be deflated first.
- Singularities and high order blocks to the eigenvalue $0, \infty$ can be deflated.
- The best treatment of infinite eigenvalue in the middle block $\lambda N_{m+1,m+1} + M_{m+1,m+1}$ is unclear.
- Is the use of skew-Cholesky better than projecting out the nullspace with unitary (symplectic) transformations?

Computational procedure

- The procedure consists of a recursive sequence of singular value decompositions.
- The staircase form essentially determines a least generic even pencil within the rounding error cloud surrounding $\lambda N + M$.
- Rank decisions face the usual difficulties and have to be adapted to the recursive procedure.
- Similar difficulties as in standard staircase form, GUPTRI.
- What to do in case of doubt? In applications, assume worst case.
- Perturbation analysis is essentially open for singular and higher order blocks associated with ∞.

Example revisited

Our MATLAB implementation of the structured staircase Algorithm determined that in the cloud of rounding-error small perturbations of each even $\lambda N + M$, there is an even pencil with structured staircase form

$$\lambda \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

with one block $\mathcal{I}_3$ with sign-characteristic 1.
The algorithm successfully located a least generic even pencil within the cloud.

Outline

Equivalence for matrix polynomials

Definition

Two $m \times n$ matrix polynomials $P(\lambda), Q(\lambda)$ are said to be equivalent, denoted $P(\lambda) \sim Q(\lambda)$, if there exist unimodular matrix polynomials $E(\lambda)$ and $F(\lambda)$ of size $m \times m$ and $n \times n$, respectively, such that

$$E(\lambda)P(\lambda)F(\lambda) = Q(\lambda).$$

The canonical form of a matrix polynomial $P(\lambda)$ under equivalence transformations is the Smith form of $P(\lambda)$.

Theorem (Smith form)

Let $P(\lambda)$ be an $m \times n$ matrix polynomial over an arbitrary field $\mathbb{F}$. Then there exists $r \in \mathbb{N}$, and unimodular matrix polynomials $E(\lambda)$ and $F(\lambda)$ of size $m \times m$ and $n \times n$, respectively, such that

$$E(\lambda)P(\lambda)F(\lambda) = \operatorname{diag}(d_1(\lambda), \ldots, d_{\min\{m,n\}}(\lambda)) =: D(\lambda),$$

where $d_1(\lambda), \ldots, d_r(\lambda)$ are monic i.e., the highest degree terms all have coefficient 1, $d_{r+1}(\lambda), \ldots, d_{\min\{m,n\}}(\lambda)$ are identically zero, and $d_j(\lambda)$ is a divisor of $d_{j+1}(\lambda)$ for $j = 1, \ldots, r-1$. Moreover, $D(\lambda)$ is unique.

The r nonzero diagonal elements $d_j(\lambda)$ in the Smith form are called the invariant polynomials or invariant factors of $P(\lambda)$.

Greatest common divisors

- For an $m \times n$ matrix A, let $\alpha \subseteq \{1, \ldots, m\}$ and $\beta \subseteq \{1, \ldots, n\}$ be arbitrary index sets of cardinality $j \leq \min(m, n)$. Then $A_{\alpha\beta}$ denotes the $j \times j$ submatrix of A in rows α and columns β; the determinant $\det A_{\alpha\beta}$ is called the $\alpha\beta$-minor of order j of A.
- For $d(x) \neq 0$, it is standard notation to write $d(x) \,|\, p(x)$ to mean that $d(x)$ is a divisor of $p(x)$, i.e., there exists some $q(x)$ such that $p(x) = d(x)q(x)$.
- Note that $d(x) \,|\, 0$ is true for any $d(x) \neq 0$. Extending this notation to a set S of scalar polynomials, we write $d \,|\, S$ to mean that $d(x)$ divides each element of S, i.e., $d(x)$ is a common divisor of the elements of S.
- The greatest common divisor (or GCD) of a set S containing at least one nonzero polynomial is the unique monic polynomial $g(x)$ such that $g(x) \,|\, S$, and if $d(x) \,|\, S$ then $d(x) \,|\, g(x)$.

Characterization of invariant polynomials

Theorem

Let $P(\lambda)$ be an $m \times n$ matrix polynomial over a field $\mathbb{F}$ with a given Smith form. Set $p_0(\lambda) \equiv 1$. For $1 \leq j \leq \min(m, n)$, let $p_j(\lambda) \equiv 0$ if all minors of $P(\lambda)$ of order j are zero; otherwise, let $p_j(\lambda)$ be the greatest common divisor of all minors of $P(\lambda)$ of order j. Then the number r in Smith form is the largest integer such that $p_r(\lambda) \not\equiv 0$. Furthermore, the invariant polynomials $d_1(\lambda), \ldots, d_r(\lambda)$ of $P(\lambda)$ are ratios of GCDs given by

$$d_j(\lambda) = \frac{p_j(\lambda)}{p_{j-1}(\lambda)}, \quad j = 1, \ldots, r,$$

the remaining diagonal entries are given by

$$d_j(\lambda) = p_j(\lambda) \equiv 0, \quad j = r+1, \ldots, \min\{m, n\}.$$

Elementary divisors

- When the field $\mathbb{F}$ is algebraically closed, the invariant polynomials are unique products of powers of linear factors

$$d_i(\lambda) = (\lambda - \lambda_{i,1})^{\alpha_{i,1}} \cdots (\lambda - \lambda_{i,k_i})^{\alpha_{i,k_i}}, \qquad i = 1, \ldots, r,$$

  where $\lambda_{i,1}, \ldots, \lambda_{i,k_i} \in \mathbb{F}$ are distinct and $\alpha_{i,1}, \ldots, \alpha_{i,k_i} \in \mathbb{N}$.
- The factors $(\lambda - \lambda_{i,j})^{\alpha_{i,j}}$, $j = 1, \ldots, k_i$, $i = 1, \ldots, r$ are called the elementary divisors of $P(\lambda)$.
- Some polynomials $(\lambda - \lambda_0)^{\alpha}$ may occur multiple times as elementary divisors of $P(\lambda)$, because they may be factors in distinct invariant polynomials $d_{i_1}(\lambda)$ and $d_{i_2}(\lambda)$.
- For a matrix $A \in \mathbb{C}^{n \times n}$, each elementary divisor $(\lambda - \lambda_0)^{\alpha}$ of the matrix pencil $\lambda I - A$ corresponds to a Jordan block of size $\alpha \times \alpha$ associated with the eigenvalue λ_0 of A.

Definition (Jordan structure of a matrix polynomial)

For an $m \times n$ matrix polynomial $P(\lambda)$ over the field $\mathbb{F}$, the Jordan structure of $P(\lambda)$ is the collection of all the finite and infinite elementary divisors of $P(\lambda)$, including repetitions, where $P(\lambda)$ is viewed as a polynomial over the algebraic closure $\overline{\mathbb{F}}$.

Companion linearization

The classical companion linearization for polynomial eigenvalue problems

$$P(\lambda)x = \sum_{i=0}^{k} \lambda^i A_i x$$

is

$$L(\lambda) = \lambda \begin{bmatrix} A_k & 0 & \cdots & 0 \\ 0 & I_n & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & I_n \end{bmatrix} + \begin{bmatrix} A_{k-1} & A_{k-2} & \cdots & A_0 \\ -I_n & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & -I_n & 0 \end{bmatrix}.$$

Companion matrix

If $P(\lambda)$ is regular and A_k invertible then we form the companion matrix

$$C_P = \begin{bmatrix} A_k^{-1}A_{k-1} & A_k^{-1}A_{k-2} & \cdots & A_k^{-1}A_0 \\ -I_n & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & -I_n & 0 \end{bmatrix}.$$

We have

$$\det P(\lambda) = \det(\lambda I + C_P)\det(A_k).$$

Theorem

For every complex number λ that is not an eigenvalue of the regular $n \times n$ matrix polynomial $P(\lambda)$ with nonsingular leading coefficient

$$P(\lambda)^{-1} = S_1(\lambda I + C_P)^{-1} T_1$$

where

$$S_1 = \begin{bmatrix} 0 & \dots & 0 & I_n \end{bmatrix}, \; T_1 = \begin{bmatrix} A_k^{-1} \\ \vdots \\ 0 \end{bmatrix}$$

Any triple (S, C, T) such that $S = S_1 M$, $C = M^{-1} C_P M$, $T = M^{-1} T_1$ is called a standard triple and we have

$$P(\lambda)^{-1} = S(\lambda I + C)^{-1} T.$$

Canonical form of linearization

Lemma

Let (S, C, T) be a standard triple for an $n \times n$ matrix polynomial $P(\lambda)$ with nonsingular leading coefficient, then

$$Q = \begin{bmatrix} SC^{k-1} \\ \vdots \\ SC \\ S \end{bmatrix}$$

is invertible and $C_P = QCQ^{-1}$

A standard triple that brings C_P to Jordan form is called a Jordan triple.

Jordan triples and matrix equations

The blocks of Jordan triples are constructed from the Jordan chains of $P(\lambda)$ and if (S, C, T) is a Jordan triple then the matrix equation

$$A_k^{-1} A_{k-1} S C^k + \ldots A_k^{-1} A_1 S C + A_k^{-1} A_0 S = 0$$

holds.

Lemma

Suppose that $D(\lambda) = \operatorname{diag}\big(d_1(\lambda), d_2(\lambda), \ldots, d_n(\lambda)\big)$ *is the Smith form of the* T*-even* $n \times n$ *matrix polynomial* $P(\lambda)$*. Then the following statements hold:*

a) *Each* $d_\ell(\lambda)$ *is alternating.*

b) *If* $P(\lambda)$ *is regular, and* ν *is the number of indices* ℓ *for which the invariant polynomial* $d_\ell(\lambda)$ *is odd, then* ν *is even.*

Theorem (Jordan struct. of T-altern. matrix poly's)

Let $P(\lambda)$ be an $n \times n$ T-alternating matrix polyn. of degree k. Then the Jordan structure of $P(\lambda)$ is as follows.

(a) *If $(\lambda - \lambda_0)^{\alpha_1}, \ldots, (\lambda - \lambda_0)^{\alpha_\ell}$ are the elem. div. to $\lambda_0 \neq 0$, then the elem. div. to $-\lambda_0$ are $(\lambda + \lambda_0)^{\alpha_1}, \ldots, (\lambda + \lambda_0)^{\alpha_\ell}$.*

(b) *Zero elementary divisors λ^β:*

- (i) *if $P(\lambda)$ is T-even, then for each odd $\beta \in \mathbb{N}$, λ^β has even multip.*
- (ii) *if $P(\lambda)$ is T-odd, then for each even $\beta \in \mathbb{N}$, λ^β has even multip.*

(c) *Infinite elementary divisors:*

- (i) *Suppose $P(\lambda)$ is T-even and k is even, or $P(\lambda)$ is T-odd and k is odd. Then $\mathrm{rev}P(\lambda)$ is T-even, and for each odd $\gamma \in \mathbb{N}$, the inf. elem. div. of $P(\lambda)$ of degree γ has even multiplicity.*
- (ii) *Suppose $P(\lambda)$ is T-even and k is odd, or $P(\lambda)$ is T-odd and k is even. Then $\mathrm{rev}P(\lambda)$ is T-odd, and for each even $\gamma \in \mathbb{N}$, the inf. elem. div. of $P(\lambda)$ of degree γ has even multiplicity.*

Corollary

Let $L(\lambda) = \lambda X + Y$ be an $n \times n$ T-alternating pencil. Then the Jordan structure of $L(\lambda)$ has the following properties:

(a) *Nonzero elementary divisors occur in pairs: if $(\lambda - \lambda_0)^{\alpha_1}, \ldots, (\lambda - \lambda_0)^{\alpha_\ell}$ are the elem. div. of $L(\lambda)$ to $\lambda_0 \neq 0$, then the elem. div. of $L(\lambda)$ to $-\lambda_0$ are $(\lambda + \lambda_0)^{\alpha_1}, \ldots, (\lambda + \lambda_0)^{\alpha_\ell}$.*

(b) *If $L(\lambda)$ is T-even, then the following elem. div. occur with even multip.*

- (i) *for each odd $\beta \in \mathbb{N}$, the elem. div. λ^β, and*
- (ii) *for each even $\gamma \in \mathbb{N}$, the elem. div. at ∞ of degree γ.*

(c) *If $L(\lambda)$ is T-odd, then the following elem. div. occur with even multi.:*

- (i) *for each even $\beta \in \mathbb{N}$, the elem. div. λ^β, and*
- (ii) *for each odd $\gamma \in \mathbb{N}$, the elem. div. at ∞ of degree γ.*

Example

Consider the T-even matrix polynomial

$$P(\lambda) = \lambda^2 \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \operatorname{diag}(\lambda^2, -1)$$

Both $P(\lambda)$ and $\operatorname{rev}P(\lambda) = \operatorname{diag}(1, -\lambda^2)$ have the same Smith form $\operatorname{diag}(1, \lambda^2)$; thus $P(\lambda)$ has elementary divisor λ^2 with odd multiplicity, and also an even degree elementary divisor at ∞ with odd multiplicity.
But this Jordan structure is incompatible with every T-even pencil. and with every T-odd pencil. Thus we see a reason why $P(\lambda)$ can have no T-alternating strong linearization.

Consequences, Questions.

- The Jordan structure of any *odd* degree T-alternating matrix polynomial $P(\lambda)$ is completely compatible with that of a T-alternating pencil of the same parity.
- This strongly suggests that it should be possible to construct a structure-preserving strong linearization for any such $P(\lambda)$.
- A question is whether compatibility of Jordan structures is also sufficient to imply the existence of a T-alternating strong linearization.
- A more refined question concerns the existence of T-alternating linearizations that preserve all the spectral information of $P(\lambda)$, comprised not only of its finite and infinite elementary divisors, but also (when $P(\lambda)$ is singular) of its Kronecker indices. See De Teran, Dopico Mackey 201x

Generalization of (Antoniou and Vologiannidis 2004).

Lemma

Let $P(\lambda)$ be any $n \times n$ matrix polynomial of odd degree, regular or singular, over an arbitrary field $\mathbb{F}$. Then $\mathcal{S}_P(\lambda)$ is a strong linearization for $P(\lambda)$.

Theorem

Every T-alternating polynomial $P(\lambda)$ of odd degree has a T-alternating strong linearization with the same parity as P.

Consequences, Questions

- We know already that there are even degree T-alternating matrix polynomials that, because of Jordan structure incompatibilities, do not have any T-alternating strong linearization.
- If we put such cases aside, however, and consider only T-alternating matrix polynomials whose Jordan structure is compatible with at least some type of T-alternating pencil, then is that compatibility sufficient to guarantee the existence of a T-alternating strong linearization? This is partially open.

Theorem

Let $P(\lambda)$ be a regular $n \times n$ T-alternating matrix polynomial of even degree $k \geq 2$, over the field $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$.

(a) *If $P(\lambda)$ is T-even, then $P(\lambda)$ has*

- *a T-even strong linearization if and only if for each even $\gamma \in \mathbb{N}$, the infinite elementary divisor of degree γ occurs with even multiplicity.*
- *a T-odd strong linearization if and only if for each even $\beta \in \mathbb{N}$, the elementary divisor λ^β occurs with even multiplicity.*

(b) *If $P(\lambda)$ is T-odd, then $P(\lambda)$ has*

- *a T-even strong linearization if and only if for each odd $\beta \in \mathbb{N}$, the elementary divisor λ^β occurs with even multiplicity.*
- *a T-odd strong linearization if and only if for each odd $\gamma \in \mathbb{N}$, the infinite elementary divisor of degree γ occurs with even multiplicity.*

Palindromic polynomials

Mackey, Mackey, Mehl, M., 2010

- Many of the results for the even case carry over to the palindromic case.
- The smith form of a T palindromic
- But there are differences, these have to do with the difference between grade and degree. $\lambda^2 I + \lambda I$ is not palindromic as a degree 2 but as degree 3 matrix polynomial.
- We don't have if and only if results.
- Many open questions.

Outline

Wilkinson Backward Error Analysis

Consider a set of data D, a computational problem and a solution space S. Suppose that the exact solution is described by mapping ϕ that maps the data $d \in D$ to a solution $s \in S$.

$$\begin{aligned} \phi &: D \to S \\ & \quad d \mapsto s \end{aligned}$$

In finite precision arithmetic we have an inaccurate solution $\tilde{\phi}$ and get an inaccurate answer $\tilde{s}$.

Wilkinson Backward Error Analysis

- Classical Wilkinson backward error analysis. Show that $\tilde{s} = \phi(\tilde{d})$, i.e. the result is the exact result with perturbed data $\tilde{d}$ and an equivalent backward error $\eta = \tilde{d} - d$.
- Then analyse via perturbation analysis what the effect of a perturbation of the data on the result is.
- The amplification factor for the error in the data is called the condition number.

Backward error analysis for $P(\lambda)x = 0$.

- Data: coefficients $A_i, i = 0, \ldots, k$.
- Solution: λ, x.
- Method: Eigenvalue solver.

For the perturbation analysis we have to analyze how the eigenvalues λ and the eigenvectors x behave under perturbation of the coefficients $A_i, i = 0, \ldots, k$, i.e. we have to determine the condition number.

Linearization

- We do not solve $P(\lambda)x = 0$, but $L(\lambda)z = 0$, where the last part of the vector z is x.
- Is the condition number of $P(\lambda)x = 0$ and $L(\lambda)z = 0$ different?
- If yes can we make the difference better by choosing different linearizations?
- What about structure preservation, does that help?

Definition

Let λ be a simple nonzero finite eigenvalue of $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$ and let x, y be the associated right and left eigenvectors. The norm-wise condition number (with respect to perturbations $\Delta P = \sum_{i=0}^{k} \lambda^i \Delta A_i$) is defined as

$$\kappa_P(\lambda) = \limsup_{\epsilon \to 0} \left\{ \frac{|\Delta\lambda|}{\epsilon|\lambda|} : (P + \Delta P)(\lambda + \Delta\lambda)(x + \Delta x) = 0, \right.$$
$$\left. \|\Delta A_i\| \leq \epsilon \omega_i, i = 0, 1, \ldots, k \right\}$$

where the weights ω_i allow to put different measures on the coefficients.

Introduce homogeneous coordinates and write
$P(\alpha,\beta) = \sum_{i=0}^{k} \alpha^i \beta^{k-i} A_i$ with $\lambda \sim \alpha/\beta$, $0 \sim (0,1)$, $\infty \sim (1,0)$.

Theorem (Dedieu/Tisseur 2003)

Let (α,β) be a simple eigenvalue of $P(\alpha,\beta)$ and let x, y be the associated right and left eigenvectors.
The norm-wise condition number (with respect to perturbations $\Delta P = \sum_{i=0}^{k} \alpha^i \beta^{k-i} \Delta A_i$) is

$$\kappa_P(\alpha,\beta) = \left(\sum_{i=0}^{k} |\alpha|^{2i} |\beta|^{2(k-i)} w_i^2 \right)^{1/2} \frac{\|x\|_2 \|y\|_2}{|y^H (\bar{\beta} \frac{d}{d\alpha} P - \bar{\alpha} \frac{d}{d\beta} P)|_{(\alpha,\beta)} x|}$$

The condition number is independent of the scaling in (α,β) and it reduces to the Wilkinson condition number for linear evps.

Conditioning of product maps

- Our solution map

$$\begin{aligned} \phi &: D \to S \\ & \quad d \mapsto s \end{aligned}$$

  is actually composed as $\phi = \phi_2(\phi_1(d))$ where ϕ_1 describes the linearization and ϕ_2 the solution of the linearized problem.
- If one of the maps ϕ_i is highly ill-conditioned then so is the product map, even if ϕ is well-conditioned.
- Usually the linearization itself is harmless computationally, so we need to analyze the conditioning of the linearization $L(\alpha, \beta) = \alpha X + \beta Y$.

Let

$$\Lambda_{\alpha,\beta} = [\alpha^{k-1}, \alpha^{k-2}\beta, \ldots, \beta^{k-1}]^T, \; w = \bar{\Lambda}_{\alpha,\beta} \otimes y, \; z = \Lambda_{\alpha,\beta} \otimes x$$

Theorem (Higham/Mackey/Tisseur 2006)

Let (α, β) be a simple eigenvalue of P with right and left eigenvectors x, y, respectively.
Then for any pencil $L(\alpha, \beta) = \alpha X + \beta Y \in \mathbb{DL}(P)$ that is a linearization of P, with ansatz vector v,

$$\kappa_L(\alpha, \beta, v) = \frac{\sqrt{|\alpha|^2\omega_X^2 + \|\beta|^2\omega_Y^2}}{|p(\alpha, \beta; v)|} \frac{\|\Lambda_{\alpha,\beta}\|\|x\|_2\|y\|_2}{|y^H(\bar{\beta}\frac{d}{d\alpha}P - \bar{\alpha}\frac{d}{d\beta}P)|_{(\alpha,\beta)}x|}$$

Optimizing the cond. number

Choose the weights $\omega_X = \|X\|_2,\ \omega_y = \|Y\|_2$ and set

$$\rho = \frac{\max_i \|A_i\|_2}{\min(\|A_0\|_2, \|A_k\|_2)}$$

Theorem

Let (α, β) be a simple eigenvalue of P with right and left eigenvectors x, y, respectively.
Then for any pencil $L(\alpha, \beta) = \alpha X + \beta Y \in \mathbb{DL}(P)$ that is a linearization of P:

$$\kappa_L(\alpha, \beta, e_1) \leq \rho k^{3/2} \inf_v \kappa_L(\alpha, \beta, v), \text{ if } A_0 \text{ is nonsing. and } |\alpha| \geq |\beta|;$$

$$\kappa_L(\alpha, \beta, e_k) \leq \rho k^{3/2} \inf_v \kappa_L(\alpha, \beta, v), \text{ if } A_k \text{ is nonsing. and } |\alpha| \leq |\beta|.$$

Thus always one e_1 or e_k will a be an almost optimal choice.

Definition

Let λ be a simple nonzero finite eigenvalue of $P(\lambda) = \sum_{i=0}^{k} \lambda^i A_i$ and let x, y be the associated right and left eigenvectors.
The norm-wise backward error (with respect to perturbations $\Delta P = \sum_{i=0}^{k} \lambda^i \Delta A_i$) is defined as

$$\begin{aligned} \eta_P(\lambda) &= \min \{\epsilon : (P + \Delta P)(\lambda)x = 0, \\ &\qquad \|\Delta A_i\| \leq \epsilon \|A_i\|, i = 0, 1, \ldots, k.\} \end{aligned}$$

Theorem (Tisseur 2001)

Let λ be a simple finite eigenvalue of $P(\lambda)$ and let x, y be the associated right and left eigenvectors.
The backward errors then are

$$\eta_P(\lambda, x) = \frac{\|P(\lambda)x\|_2}{(\sum_{i=0}^{k} |\lambda^i| \|A_i\|_2)\|x\|_2}$$

$$\eta_P(y^H, \lambda) = \frac{\|y^H P(\lambda)\|_2}{\|y\|_2(\sum_{i=0}^{k} |\lambda^i| \|A_i\|_2)}$$

Theorem (Higham, Li, Tisseur 2007)

Let λ be a simple finite eigenvalue of $P(\lambda)$ and let x, y be the associated right and left eigenvectors.
The backward errors then are

$$\eta_P(\alpha, \beta, x) = \frac{\|P(\alpha, \beta)x\|_2}{(\sum_{i=0}^{k} |\alpha^i||\beta^{k-i}|\|A_i\|_2)\|x\|_2}$$

$$\eta_P(y^H, \alpha, \beta) = \frac{\|y^H P(\alpha, \beta)\|_2}{\|y\|_2(\sum_{i=0}^{k} |\alpha^i||\beta^{k-i}|\|A_i\|_2)}$$

Theorem (Higham, Li, Tisseur 2007)

Let (α, β) be a simple eigenvalue of a regular $P(\alpha, \beta)$ and let x be the associated right eigenvector. Let $L(\alpha, \beta) \in \mathbb{DL}(P)$ be a linearization with unit norm ansatz vector v with r nonzeros and let z be the corresponding ev. of L.
Then

$$\frac{\eta_P(\alpha,\beta,x)}{\eta_L(\alpha,\beta,z)} \leq kr^{1/2}\frac{(|\alpha|+|\beta|)\|\Lambda_{\alpha,\beta}\|\max_i \|A_i\|_2\|z\|_2}{\sum_{i=0}^{k}|\alpha^i||\beta^{k-i}|\|A_i\|_2)\|x\|_2} \leq k^{3/2}r^{1/2}\rho\frac{\|z\|_2}{\|x\|_2}$$

Scaling

Consider a quadratic polynomial $P(\lambda) = \lambda^2 A + \lambda B + C$ and let

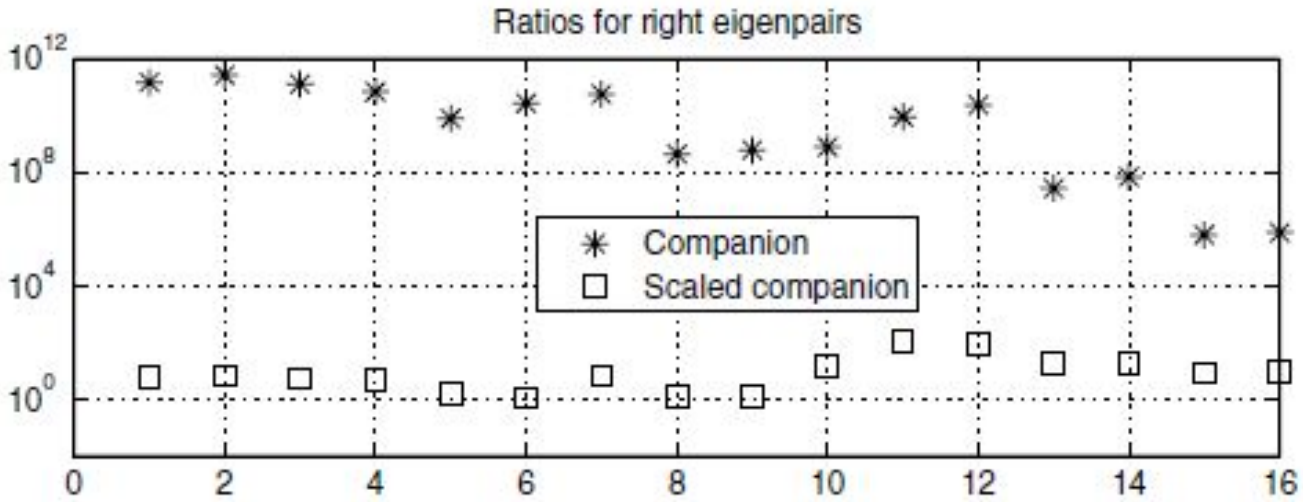
$$a = \|A\|, \; b = \|B\|, \; c = \|C\|$$

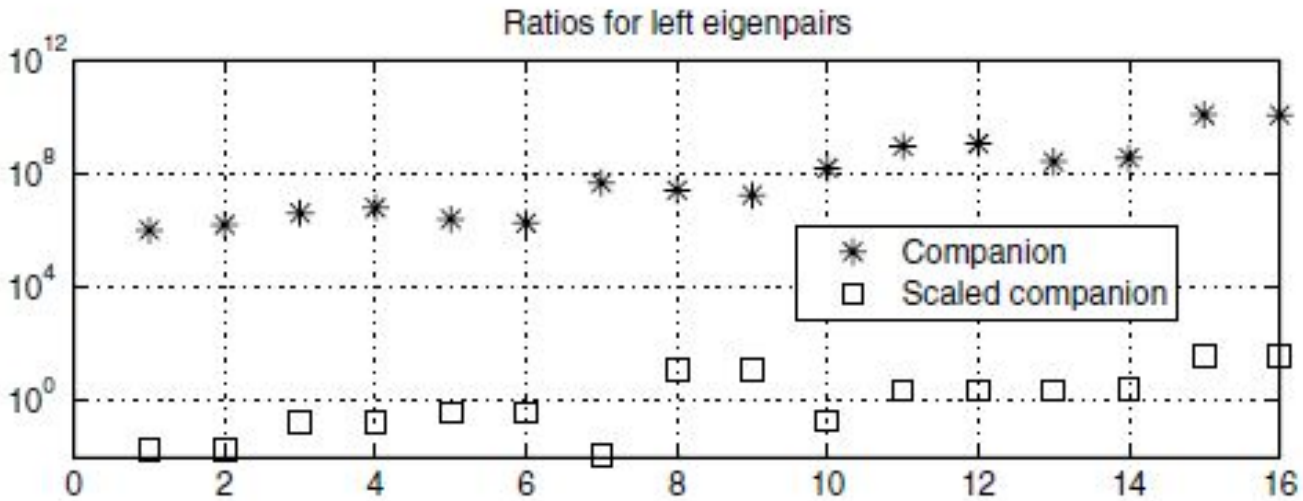
and choose $\gamma = \sqrt{c/a}$. Then with $\lambda = \mu\gamma$ it was shown in Fan, Lin, Van Dooren 2004

$$P(\lambda) = \mu^2(\gamma^2)A + \mu(\gamma B) + C$$

that this choice of γ is the choice that minimizes ρ.

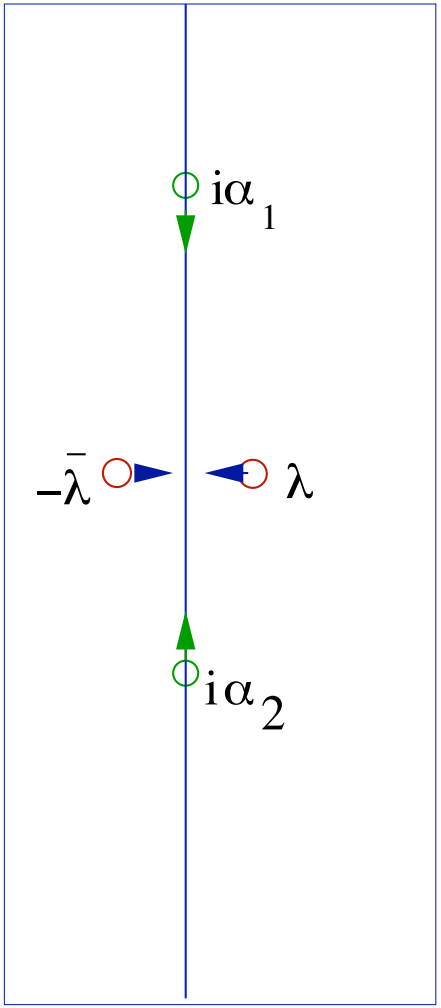
Ratios of backward error η_P/η_{C_1}



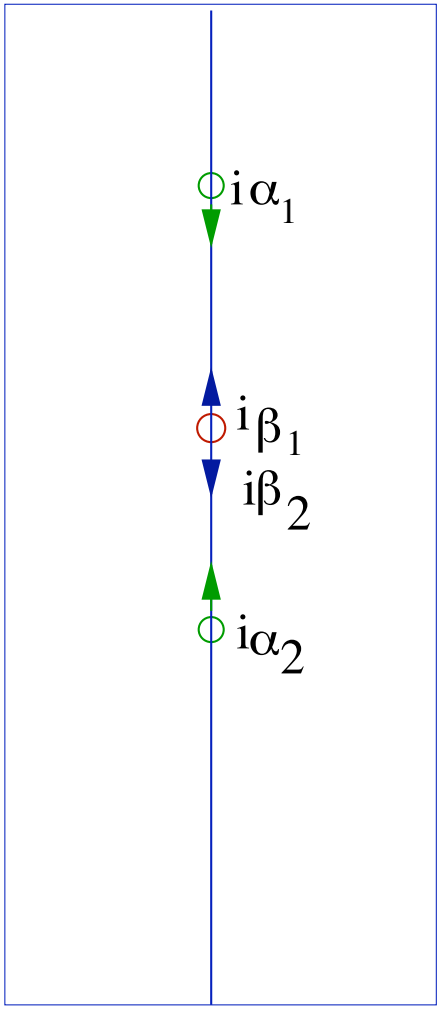


Structured vs. unstructured perturb.

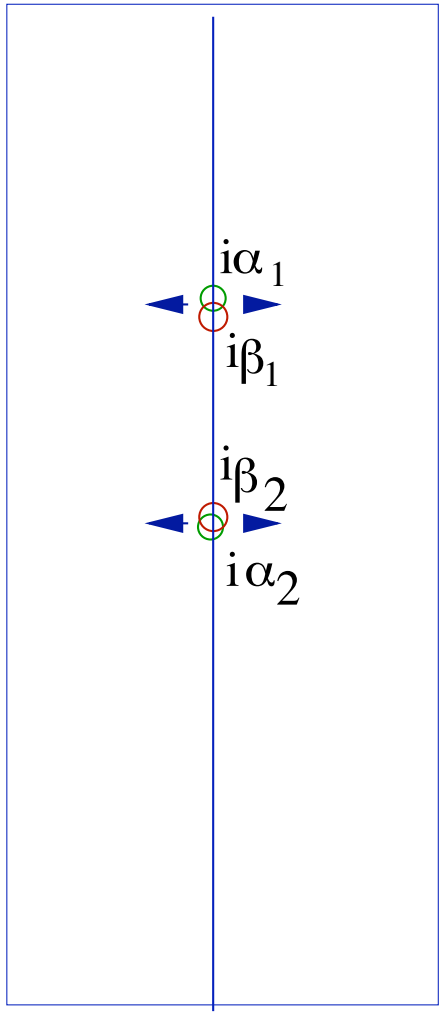
- Structured condition numbers are typically less than or equal than the unstructured ones. See Adhikari/Alam 2009, Ahmad/Mehmann 2010.
- The structured backward errors are typically less than or equal than the unstructured ones.
- The formulas are pretty ugly.
- Examples are difficult. Consider a 4×4 even pencil with two purely imaginary eigenvalues $i\alpha_1, i\alpha_2$ and eigenvalues $\lambda, -\bar{\lambda}$, with nonzero real part.



(1)



(2)



(3)

Outline

Typical questions

- Find all eigenvalues λ and associated eigenvectors x for a given parameter value α.
- Find some important eigenvalues λ and associated eigenvectors x for a given parameter α.
- Find all eigenvalues in a given subset of $\mathbb{C}$ for a given parameter α.
- Optimize eigenvalue positions over parameter set.
- ....

Small scale problems

Small scale problems n several 1000, compute all the eigenvalues.

- QR algorithm (LAPACK, MATLAB (eig),...) for $P(\lambda) = \lambda I - A$
- QZ algorithm (LAPACK, MATLAB (eig) ,...) for $P(\lambda) = \lambda A_1 + A_0$ regular, square.
- GUPTRI for $P(\lambda) = \lambda A_1 + A_0$ general.
- QZ, GUPTRI algorithm (LAPACK, MATLAB (polyeig),...) for $P(\lambda) = \sum_{i=0}^{k} \lambda^i A^i$ via linearization.

The QZ algorithm

Given a regular pencil $\lambda A_1 + A_0$

- First determine unitary/orthogonal P, Q such that $PA_1Q = T_1$ is upper triangular and $PA_0Q = H_0$ is upper Hessenberg.
- Deflate eigenvalues ∞
- Apply implicitly the QR algorithm to the upper Hessenberg matrix $T_1^{-1}H_0$ without ever forming it.
- After convergence we have $PA_1Q = T_1$ and $PA_0Q = T_0$ (quasi)-upper triangular.

Recent developments

- Aggressive deflation, block orientation. Kågström/Kressner 2006-2008
- New Lapack version
- High performance versions in Scalapack ?
- As long as there is enough storage, it can be applied to full dense matrices of dimension several 10000.

Summary full dense methods

- Good linearization plus full dense QZ algorithm solves many problems.
- As a quick solution it may be the best to do.
- For larger problems polyeig, or a good linearization and eigs are good choices.
- Special methods for even and palindromic pencils

Newton's method

Consider $P(\lambda)x = 0$ where P is an arbitrary matrix function.
Kublanovskaya 1969: Use a QR-decomposition with column pivoting $P(\lambda)\Pi(\lambda) = Q(\lambda)R(\lambda)$, where $\Pi(\lambda)$ is such that $|r_{11}(\lambda)| \geq |r_{22}(\lambda)| \geq \cdots \geq |r_{nn}(\lambda)|$.
Then λ is an eigenvalue if and only if $r_{nn}(\lambda) = 0$.
Applying Newton's method, one obtains

$$\lambda_{k+1} = \lambda_k - \frac{1}{e_n^H Q(\lambda_k)^H P'(\lambda_k)\Pi(\lambda_k)R(\lambda_k)^{-1}e_n}$$

for approximations to an eigenvalue.
Approximations to left and right eigenvectors can be obtained from

$$y_k = Q(\lambda_k)e_n \quad \text{and} \quad x_k = \Pi(\lambda_k)R(\lambda_k)^{-1}e_n.$$

Analysis

- Method converges quadratically.
- This relatively simple idea is not efficient, since it computes eigenvalues one at a time and needs several $\mathcal{O}(n^3)$ factorizations per eigenvalue.
- It is, however, useful in the context of iterative refinement of computed eigenvalues and eigenvectors.

Nonlinear inverse iteration

- For $Ax = \lambda x$ inverse iteration is equivalent to Newton's method for

$$\begin{bmatrix} Ax - \lambda x \\ v^H x - 1 \end{bmatrix} = 0,$$

where $v \in \mathbb{C}^n$ is suitably chosen.

- For the nonlinear problem

$$\begin{bmatrix} P(\lambda)x \\ v^H x - 1 \end{bmatrix} = 0$$

one step of Newton's method gives

$$\begin{bmatrix} P(\lambda_k) & P'(\lambda_k)x_k \\ v^H & 0 \end{bmatrix} \begin{bmatrix} x_{k+1} - x_k \\ \lambda_{k+1} - \lambda_k \end{bmatrix} = - \begin{bmatrix} P(\lambda_k)x_k \\ v^H x_k - 1 \end{bmatrix}.$$

- This gives $u_{k+1} := P(\lambda_k)^{-1} P'(\lambda_k)x_k$. and with $v^H x_{k+1} = v^H x_k$, then $\lambda_{k+1} = \lambda_k - \frac{v^H x_k}{v^H u_{k+1}}$.

Inverse iteration

1: Start with λ_0, x_0 such that $v^H x_0 = 1$
2: **for** $k = 0, 1, 2, \ldots$ until convergence **do**
3: solve $P(\lambda_k)u_{k+1} = P'(\lambda_k)x_k$ for u_{k+1}
4: $\lambda_{k+1} = \lambda_k - (v^H x_k)/(v^H u_{k+1})$
5: normalize $x_{k+1} = u_{k+1}/v^H u_{k+1}$
6: **end for**

Analysis

- This algorithm is a variant of Newton's method. It converges locally and quadratically to some (x, λ).
- It was suggested by Ruhe 1973 to use $v_k = P(\lambda_k)^H y_k$ for the normalization, where y_k is an approximation to a left ev.
- Then the update for λ becomes

$$\lambda_{k+1} = \lambda_k - \frac{y_k^H P(\lambda_k) x_k}{y_k^H P'(\lambda_k) x_k},$$

  which is the nonlinear Rayleigh functional Lancaster 2002.
- This functional can be interpreted as one Newton step for solving the equation $f_k(\lambda) := y_k^H P(\lambda) x_k = 0$.
- For linear Hermitian problems this gives cubic convergence if λ_k is updated by the Rayleigh quotient Crandall 1951.
- The same holds for symmetric nonlinear problems if we set in Step 4 $\lambda_{k+1} = p(u_{k+1})$, where $p(u_{k+1})$ denotes the real root of $u_{k+1}^H P(\lambda) u_{k+1} = 0$ closest to λ_k.

Simplified Newton

- Inverse iteration needs a large number of factorizations.
- The obvious idea then is to fix the shift σ i.e. to use, $x_{k+1} = (A - \sigma I)^{-1} x_k$.
- However, in general this method does not converge in the nonlinear case.
- Neumaier 1985. Assume that $P(\lambda)$ is twice continuously differentiable, then inverse iteration gives

$$\begin{aligned} x_k - x_{k+1} &= x_k + (\lambda_{k+1} - \lambda_k) P(\lambda_k)^{-1} P'(\lambda_k) x_k \\ &= P(\lambda_k)^{-1} (P(\lambda_k) + (\lambda_{k+1} - \lambda_k) P'(\lambda_k)) x_k \\ &= P(\lambda_k)^{-1} P(\lambda_{k+1}) x_k + \mathcal{O}(|\lambda_{k+1} - \lambda_k|^2). \end{aligned}$$

- Neglecting the second order term one gets

$$x_{k+1} = x_k - P(\lambda_k)^{-1} P(\lambda_{k+1}) x_k.$$

Residual inverse iteration

1: Let v be a normalization vector and start with an approximations σ and x_1 to an eigenvalue and corresponding eigenvector such that $v^H x_1 = 1$
2: **for** $k = 1, 2, \ldots$ until convergence **do**
3: solve $v^H P(\sigma)^{-1} P(\lambda_{k+1}) x_k = 0$ for λ_{k+1}
or $x_k^H P(\lambda_{k+1}) x_k = 0$ if $P(\lambda)$ is Hermitian and λ_{k+1} is real
4: compute the residual $r_k = P(\lambda_{k+1}) x_k$
5: solve $P(\sigma) d_k = r_k$ for d_k
6: set $z_{k+1} = x_k - d_k$
7: normalize $x_{k+1} = z_{k+1} / v^H z_{k+1}$
8: **end for**

Theorem (Neumaier 1985)

If $P(\lambda)$ is twice continuously differentiable, $\hat{\lambda}$ a simple zero of $\det P(\lambda) = 0$, *and if $\hat{x}$ is an eigenvector normalized by $v^H \hat{x} = 1$, then the residual inverse iteration converges for all σ sufficiently close to $\hat{\lambda}$, and one has the estimate*

$$\frac{\|x_{k+1} - \hat{x}\|}{\|x_k - \hat{x}\|} = \mathcal{O}(|\sigma - \hat{\lambda}|) \quad \textit{and} \quad |\lambda_{k+1} - \hat{\lambda}| = \mathcal{O}(\|x_k - \hat{x}\|^q),$$

where $q = 2$ if $P(\lambda)$ is Hermitian, $\hat{\lambda}$ is real, and λ_{k+1} solves $x_k^H P(\lambda_{k+1}) x_k = 0$ in Step 3, and $q = 1$ otherwise.

Method of successive linear problems

1: Start with an approximation λ_1 to an eigenvalue
2: **for** $k = 1, 2, \ldots$ until convergence **do**
3: solve the linear eigenproblem $P(\lambda_k)u = \theta P'(\lambda_k)u$
4: choose an eigenvalue θ smallest in modulus
5: $\lambda_{k+1} = \lambda_k - \theta$
6: **end for**

Theorem (Ruhe 1973)

If P is twice continuously differentiable, and $\hat{\lambda}$ is an eigenvalue such that $P'(\hat{\lambda})$ is nonsingular and 0 is an algebraically simple eigenvalue of $P'(\hat{\lambda})^{-1}P(\hat{\lambda})$, then the method of successive linear problems converges quadratically to $\hat{\lambda}$.

Newton and inverse iteration

- The discussed Newton and inverse iteration methods can be used for general nonlinear evps.
- For Hermitian problems and real eigenvalues they converge faster if the eigenvalue approximations are updated using the Rayleigh functional.
- One typically gets only one eigenvalue/vector at a time.
- Sometimes the methods repeatedly converge to the same ev.
- Deflation is problematic.
- We do not have a guarantee that we find all eigenvalues in a given set.
- Matrix factorizations are needed to solve the linear system. With sparse solvers this can be done (if not too often) for very large sizes MUMPS, UMFPACK, PARDISO, ...

Safeguarded iteration

For Hermitian problems that allow a variational characterization of their eigenvalues we can use the safeguarded iteration Werner 1970, Voss/Werner 1982.

- Let $J \subset \mathbb{R}$ be an open interval and assume that $F(\lambda) \in \mathbb{C}^{n,n}$ is a family of Hermitian matrices, where the elements are differentiable in λ.
- Assume that for every $x \in \mathbb{C}^n \setminus \{0\}$ the real equation

$$f(\lambda, x) := x^H F(\lambda) x = 0$$

  has at most one solution $\lambda \in J$.
- Then f defines a functional ρ on some subset $D \subset \mathbb{C}^n$ called Rayleigh functional of the nonlinear evp which generalizes the Rayleigh quotient for linear pencils $F(\lambda) = \lambda A_1 + A_0$.
- Assume further that $x^H F'(\rho(x))x > 0$ for every $x \in D$ then differentiating the identity $x^H F(\rho(x))x = 0$ one obtains that the e'vecs are stationary points of ρ.

Minimax principle

Under the described assumtions a minimax principle for the nonlinear eigenproblem holds if the eigenvalues are enumerated appropriately.

- A value $\lambda \in J$ is an eigenvalue of $F(\lambda)x = 0$ if and only if $\mu = 0$ is an eigenvalue of the matrix $F(\lambda)$, and by Poincaré's max-min principle there exists $m \in \mathbb{N}$ such that

$$0 = \max_{\dim V = m} \min_{x \in V,\ x \neq 0} \frac{x^H F(\lambda) x}{\|x\|^2}.$$

- One assigns this m to λ as *its number* and calls λ an *m*-th eigenvalue of the problem.

Theorem (Voss/Werner 1982)

Under the above assumptions, for every $m \in \{1, \ldots, n\}$, $F(\lambda)x = 0$ has at most one m-th eigenvalue in J, given by

$$\lambda_m = \min_{\dim V = m, D \cap V \neq \emptyset} \sup_{v \in D \cap V} \rho(v).$$

Conversely, if

$$\lambda_m := \inf_{\dim V = m, D \cap V \neq \emptyset} \sup_{v \in D \cap V} \rho(v) \in J,$$

then λ_m is an m-th eigenvalue of $F(\lambda)x = 0$.
The minimum is attained by the invariant subspace of $F(\lambda_m)$ corresponding to its m largest eigenvalues, and the supremum is attained by any eigenvector of $F(\lambda_m)$ corresponding to $\mu = 0$.

Safeguarded iteration

The enumeration of eigenvalues and the fact that the eigenvectors are the stationary vectors of the Rayleigh functional suggests the following Algorithm.

1: Start with an approximation σ_1 to the m-th eigenvalue
2: **for** $k = 1, 2, \ldots$ until convergence **do**
3: determine an eigenvector x_k corresponding to the m-largest eigenvalue of $F(\sigma_k)$
4: solve $x_k^H F(\sigma_{k+1}) x_k = 0$ for σ_{k+1}
5: **end for**

Analysis

- If $\lambda_1 := \inf_{x \in D} \rho(x) \in J$ and $x_1 \in D$ then the iteration converges globally to λ_1.
- If $\lambda_m \in J$ is an m-th eigenvalue which is simple, then the iteration converges locally and quadratically to λ_m.
- Let $F(\lambda)$ be twice continuously differentiable, and assume that $F'(\lambda)$ is positive definite for $\lambda \in J$. If, in Step 3 of the Algorithm, x_k is chosen to be an eigenvector corresponding to the m-th largest eigenvalue of the generalized evp $F(\sigma_k)x = \mu F'(\sigma_k)x$, then the convergence is even cubic.

Evaluation

- Whenever the problem has a variational background and the eigenvalues are real this is the best method.
- One gets information about the eigenvalues that no other method provides.
- It can be easily combined with grid refinement and multilevel approaches.
- It is used in a huge number of applications with great success.
- More information and applications see H. Voss website.

Nonlinear Newton evp. solver

Nonlinear evp $F(\lambda)x = 0$. Apply Newton to function

$$f_w(x,\lambda) = \begin{bmatrix} F(\lambda)x \\ w^H x - 1 \end{bmatrix} = 0.$$

The Newton system for $\lambda_{k+1} = \lambda_k + \mu_k$ and $x_{k+1} = x_k + s_k$ is

$$\begin{bmatrix} F(\lambda_k) & F'(\lambda_k)x_k \\ w^H & 0 \end{bmatrix} \begin{bmatrix} s_k \\ \mu_k \end{bmatrix} = - \begin{bmatrix} F(\lambda_k)x_k \\ w^H x_k - 1 \end{bmatrix}$$

or

$$\begin{aligned} \lambda_{k+1} &= \lambda_k - \frac{1}{w^H F(\lambda_k)^{-1} F'(\lambda_k) x_k} \\ x_{k+1} &= (\lambda_k - \lambda_{k+1}) F(\lambda_k)^{-1} F'(\lambda_k) x_k. \end{aligned}$$

Difficulties

- In many applications we want all evs in a given set.
- How do we guarantee that we find all.
- Deflation of computed evs.
- Need to use sparse solvers.
- Need to get into convergence intervals for Newton.
- No global analysis and easy to use industrial implementation.

Finding all evs in a region R of $\mathbb{C}$

For the general case $F(\lambda)x = 0$ and most iterative methods it is an open problem to guarantee that we find all eigenvalues in a given set $R \subset \mathbb{C}$.

- We can use Bendixon's theorem or Gersgorin type results to analyze the number of eigenvalues.
- The computation can in principle be done with any solver and many start points.
- We could use the sign function method (not for large problems) or the Cauchy integral theorem (Beyn 2009).
- Homotopy or path following seem to be the only option.
- None of these methods is really satisfactory.

Homotopy

- Replace $F(\lambda)$ by $P(\lambda) + g(t)Q(\lambda)$, where the problem $P(\lambda)x = 0$ is 'easy' and where g is a monotonically increasing function of t with $g(0) = 0$, $g(1) = 1$.
- Compute all the eigenvalues $\lambda_i(0)$ of P in the given set R and possible the associated ev.
- Large potential for parallelism.
- Follow the eigenvalue curves $\lambda_i(t)$.
- Determine eigenvalues that leave R.
- Determine eigenvalues that come into R from outside.
- Determine bifurcation points.
- Use step size control to guarantee that no ev. is missed.
- Use Newton method for fully nonlinear problem.

Difficulties

- If the 'hard part' is large, then evs. move a lot.
- Small homotopy steps may be needed to track ev's of nonlinear problem.
- Many factorizations may be needed.
- Need to use out-of-core sparse solvers.
- Need to get into convergence intervals for Newton.
- Need to update search directions in a clever way to make stepsizes small.

Application to acoustic problem

Consider nonlinear eigenvalue problem $P(\lambda)x = 0$, where

$$P(\lambda) := \lambda^2 \begin{bmatrix} M_s & 0 \\ 0 & M_f \end{bmatrix} + \lambda \begin{bmatrix} D_s & D_{as}^T \\ D_{as} & D_f \end{bmatrix} + \begin{bmatrix} K_s(\lambda) & 0 \\ 0 & K_f \end{bmatrix},$$

is **complex symmetric** and has dimension up to $10,000,000$.
Goal: Compute all eigenvalues in a given region R of $\mathbb{C}$ and associated eigenvectors.

Model/modal reduction

- After desired ev's and deflating subspaces $U = [u_1, \ldots, u_k]$ have been computed, the projected system

$$U^T M(\alpha) U\ddot{z} + U^T D(\alpha) U\dot{z} + U^T K(\alpha) Uz = U^T f$$

  is formed and optimization is done on this system.
- The original decoupled projection (fluid and structure separately) does not work.
- We really need nonlinear model reduction (open problem).
- We need to use the fact that only a small part of the system is changed in every optimization step.
- We need to integrate ev computation, gradient computation, discretization.
- An adaptive multilevel approach would be great (Reduced order modeling)

Projection methods, linear evps.

- For large sparse linear evps $Ax = \lambda x$, iterative projection methods like the Lanczos, Arnoldi, rational Krylov or Jacobi–Davidson method are well established.
- Basic idea: Construction of a search space (typically a Krylov subspace) followed by projection into this subspace.
- This gives a small dense problem, handled by a dense solver and the eigenvalues of the projected problem are used as approximations.
- Main features: Matrix factorizations are avoided as much as possible (except in the context of preconditioning), and the generation of the search space is usually done via an iterative procedure that is based on matrix vector products that can be cheaply obtained.

Basic types

Two basic types:

- Methods which expand the subspaces independently of the eigenpair of the projected problem and which use Krylov subspaces of A or $(A - \sigma I)^{-1}$ for some shift σ. These methods include the Arnoldi, Lanczos or rational Krylov method.
- Methods that aim at a particular eigenpair and choose the expansion q such that it has a high approximation potential for a desired eigenvalue/eigenvector or invariant subspace. An example for this approach is the Jacobi–Davidson method.

Krylov subspace methods

- For the Arnoldi and other Krylov subspace methods, the search space is a Krylov space

$$\mathcal{K}_k(A, v_1) = \text{span}\{v_1, Av_1, A^2v_1, \ldots, A^{k-1}v_1\},$$

where v_1 is an appropriately chosen initial vector.

- Arnoldi produces an orthogonal basis V_k of $\mathcal{K}_k(A, v_1)$ such that the projected matrix H_k is upper Hessenberg and satisfies

$$AV_k = V_k H_k + f_k e_k^T,$$

where $e_k \in \mathbb{R}^k$ is the k-th unit vector and f_k is orthogonal to the columns of V_k, i.e. $V_k^H f_k = 0$.

- The orthogonality of V_k implies that $V_k^H A V_k = H_k$ is the orthogonal projection of A to $\mathcal{K}_k(A, v_1)$.

Ritz pairs

- If (y, θ) is an eigenpair of the projected problem, and $x = V_k y$ is the corresponding approximation to an eigenvector of $Ax = \lambda x$ (which is called a Ritz vector corresponding to the Ritz value θ), then the residual satisfies

$$r := Ax - \theta x = AV_k y - \theta V_k y = V_k H_k y - \theta V_k y + f_k e_k^H y = (e_k^H y) f_k.$$

- Hence, one obtains an error indicator $\|r\| = |e_k^T y| \cdot \|f_k\|$ for the eigenpair approximation (x, θ) without actually computing the Ritz vector x.
- If A is Hermitian then this is even an error bound.

Evaluation

- The Arnoldi method together with its variants, such as shift-and-invert and implicit restart, is today a standard solver.
- It is implemented in the package ARPACK and the MATLAB command eigs.
- It typically converges to the extreme eigenvalues first.
- If one is interested in eigenvalues in the interior of the spectrum, or in eigenvalues close to a given focal point τ, then one can apply the method in a shift-and-invert fashion, i.e. to the matrix $(A - \tau I)^{-1}$ or an approximation of it.
- In this case one has to determine a factorization of $A - \tau I$, which, however, may be prohibitive for very large problems.
- One may use a preconditioned iterative solver here.

Jacobi-Davidson method

An alternative is the Jacobi–Davidson method.

- Let (x, θ) be an approximation to an eigenpair obtained by a projection method with subspace V.
- We assume that $\|x\| = 1$, $\theta = x^H A x$ and $r := Ax - \theta x \perp x$.
- Then the most desirable orthogonal correction z solves the equation

$$A(x + z) = \lambda(x + z), \quad z \perp x.$$

- As $z \perp x$, the operator A can be restricted to the subspace orthogonal to x yielding $\tilde{A} := (I - xx^H)A(I - xx^H)$, and from $\theta = x^H A x$ it follows that

$$A = \tilde{A} + AxxH + xx^H A - \theta xx^H.$$

Correction equation

- Hence, $(\tilde{A} - \lambda I)z = -r + (\lambda - \theta - x^H Az)x$.
- Since both the left hand side and r are orthogonal to x, it follows that the factor $\lambda - \theta - x^H Az$ must vanish, and therefore the correction z has to satisfy $(\tilde{A} - \lambda I)z = -r$.
- Since λ is unknown, it is replaced by a Ritz approximation θ, and one ends up with the correction equation

$$(I - xx^H)(A - \theta I)(I - xx^H)z = -r.$$

- The expanded space $[V, z]$ for the Jacobi–Davidson method contains $u = (A - \theta I)^{-1}x$, obtained by one step of inverse iteration.
- One can expect similar approximation properties, i.e. quadratic or even cubic convergence, if the problem is Hermitian.
- The Jacobi–Davidson method is aiming at a particular eigenvalue (close to the shift θ).

Comparison Arnoldi, JD

- Both, the shift-and-invert Arnoldi method and the Jacobi-Davidson method have to solve a large linear system.
- In the Arnoldi method this system in general needs to be solved very accurately to get fast convergence.
- In the Jacobi–Davidson method it suffices to solve this system approximately to maintain fast convergence.
- Typically only a small number of steps of a preconditioned iterative method are sufficient to obtain a good expansion z for the search space V.
- Implementations of JD in FORTRAN and MATLAB can be downloaded from
  `http://www.math.ruu.nl/people/sleijpen`.

Struct. proj. methods

- Structure preserving linearizations plus structure preserving Arnoldi methods for linear problems are available for many structures. (Even, palindromic, . . .).
- The use of structure saves computing time and one gets more accurate results.
- One has to design specific spaces and specific projections. Apel/M./Watkins 2002, M./Schröder/Simoncini 2009.
- Many open problems.

Proj. methods for nonl. evps

Consider $F(\lambda)x = 0$.

- Expand the search space by directions that has a high approximation potential for the next desired eigenvector.
- Assume that V is an orth. basis of current search space.
- Let (θ, y) be a solution of the proj. problem $V^H F(\lambda) V y = 0$, and let $x = Vy$ be the Ritz vector.
- Two candidates for expanding V: $\hat{v} = x - F(\sigma)^{-1} F(\theta) x$ motivated by residual inverse iteration, and $\tilde{v} = F(\theta)^{-1} F'(\theta) x$ corresponding to inverse iteration.
- Expanding search space V by $\hat{v}$ results in Arnoldi type methods.
- Expanding it by $\tilde{v}$ requires the solution of a large linear system in every iteration step. This can be avoided by a Jacobi–Davidson approach .

Nonlinear Arnoldi

- We consider the expansion of V by $\hat{v} = x - F(\sigma)^{-1}F(\theta)x$, where σ is a fixed shift (not too far away from focal point).
- The new search direction is orthonormalized against the previous ansatz vectors.
- Since the Ritz vector x is contained in the span of V, one may choose the new direction $v = F(\sigma)^{-1}F(\theta)x$ as well.
- For the linear problem $F(\lambda) = A_0 + \lambda A_1$ this is exactly the Cayley transformation with pole σ and zero θ

$$(A_0 + \sigma A_1)^{-1}(A_0 + \theta A_1) = I + (\theta - \sigma)(A_0 + \sigma A_1)^{-1}A_1$$

- Krylov spaces are shift-invariant, the resulting projection method expanding V by v the shift-and-invert Arnoldi method.
- If it is too expensive to solve the linear system $F(\sigma)v = F(\theta)x$ for v, one may choose $v = MF(\theta)x$ with $M \approx F(\sigma)^{-1}$.

Nonlinear Arnoldi, Ruhe 1998

start with an initial shift σ and an initial basis V, $V^H V = I$;
determine a preconditioner $M \approx F(\sigma)^{-1}$,
for $m = 1, 2, \ldots,$ number of wanted eigenvalues **do**
    comp. ev μ and evec y of $F_V(\mu)y := V^H F(\mu) V y = 0$.
    determine Ritz vector $u = Vy$ and residual $r = F(\mu)u$
    if $\|r\|/\|u\| < \epsilon$ **then**
        accept approximate eigenpair $\lambda_m = \mu$, $x_m = u$,
        if $m ==$ number of desired eigenvalues **then** STOP **end if**
        choose new shift σ and precond. $M \approx F(\sigma)^{-1}$ if indicated
        restart if necessary
        choose approximations μ and u
        determine residual $r = F(\mu)u$
    end if
    $v = Mr$
    $v = v - VV^H v$,$\tilde{v} = v/\|v\|$, $V = [V, \tilde{v}]$
    reorthogonalize if necessary
end for

Discussion

- In Step 1 any pre-information such as known approximate eigenvectors should be used.
- If no information on eigenvectors is at hand, and one is interested in evs near $\tau \in D$, choose an initial vector at random, execute a few Arnoldi steps for the linear evp $F(\tau)u = \theta u$ or $F(\tau)u = \theta F'(\tau)u$, and choose V by orthogonalizing evecs. Starting with a random vector without this preprocessing does not lead to convergence.
- The preconditioner in Step 2 should be chosen on the basis of the underlying problem. If this is not available, then use full or incomplete sparse LU decompositions of $F(\sigma)$.
- Update the preconditioner if the convergence measured by the quotient of the last two residual norms before convergence has become too slow.

Nonlinear Jacobi–Davidson

- Suppose that the columns of $V \subset \mathbb{C}^n$ form an orthonormal basis of the current search space, and let (x, θ) be a Ritz pair i.e. $V^H F(\theta) V y = 0$, $x = Vy$.
- Consider the correction equation

$$\left(I - \frac{px^H}{x^H p}\right) F(\theta) \left(I - \frac{xx^H}{x^H x}\right) z = -r, \quad z \perp x,$$

  where $p := F'(\theta)x$ and $r := F(\theta)x$.
- Rewrite this as $F(\theta)z - \alpha p = -r$, where α has to be chosen such that $z \perp x$.
- Solving for z we obtain

$$z = -x + \alpha F(\theta)^{-1} p = -x + \alpha F(\theta)^{-1} F'(\theta) x,$$

  and $x = Vy$ yields that $\tilde{z} := F(\theta)^{-1} F'(\theta) x \in \text{span}[V, z]$.

Discussion

- The new search space span$[V, z]$ contains the vector obtained by one step of inverse iteration with shift θ and initial vector x
- We expect quadratic or even cubic convergence, if the correction equation is solved exactly.
- Usually a few steps of a Krylov solver with an appropriate preconditioner suffice to obtain a good expansion direction.
- If a Krylov solver is used and the initial approximation is orthogonal to x then all iterates are orthogonal to x as well.
- The operator $F(\theta)$ is restricted to map the subspace $x^{\perp}$ to $(F'(\theta)x)^{\perp}$.
- If $K \approx F(\theta)$ is a preconditioner of $F(\theta)$ then a preconditioner for an iterative solver is

$$\tilde{K} := (I - \frac{px^H}{x^H p})K(I - \frac{xx^H}{x^H x}).$$

Template

start with an initial shift σ and an initial basis V, $V^H V = I$;
determine a preconditioner $M \approx \mathcal{F}(\sigma)^{-1}$,
for $m = 1, 2, \ldots,$ number of wanted eigenvalues **do**
  compute ev μ and evec y of $\mathcal{F}_V(\mu)y := V^H \mathcal{F}(\mu) V y = 0$.
  determine Ritz vector $u = Vy$ and residual $r = \mathcal{F}(\mu)u$
  if $\|r\|/\|u\| < \epsilon$ **then**
    accept approximate eigenpair $\lambda_m = \mu$, $x_m = u$,
    if $m ==$ number of desired evs **then** STOP **end if**
    choose new shift σ and a precond. $M \approx \mathcal{F}(\sigma)^{-1}$
    restart if necessary
    choose approx. μ and u
    determine residual $r = \mathcal{F}(\mu)u$
  end if
  Find an appr. solution of $(I - \frac{F'(\mu)uu^H}{u^H F'(\mu)u})F(\mu)(I - \frac{uu^H}{u^H u})t = -r$
  $v = v - VV^H v$,$\tilde{v} = v/\|v\|$, $V = [V, \tilde{v}]$
  reorthogonalize if necessary
end for

Idea of Rat. Krylov

- Linearize the nonlinear family $F(\lambda)$ by Lagrange interpolation between two points μ and σ.

$$F(\lambda) = \frac{\lambda - \mu}{\sigma - \mu} F(\sigma) + \frac{\lambda - \sigma}{\mu - \sigma} F(\mu) + \text{higher order terms.}$$

- Keep σ fixed for several steps, iterate on μ, neglect the remainder in the Lagrange interpolation, and multiply by $F(\sigma)^{-1}$ from the left:

$$F(\sigma)^{-1} F(\lambda_{j-1}) w = \theta w \quad \text{with} \quad \theta = \frac{\lambda_j - \lambda_{j-1}}{\lambda_j - \sigma},$$

- This predicts a singularity at

$$\lambda_j = \lambda_{j-1} + \frac{\theta}{1 - \theta}(\lambda_{j-1} - \sigma).$$

- For large and sparse matrices combine with linear Arnoldi process.

- After j steps, approx. evs $\lambda_1, \ldots, \lambda_j$, orthon. $V_j = [v_1, \ldots, v_j]$, and upper Hessenb. $H_{j,j-1} \in \mathbb{C}^{j,j-1}$ are generated, with

$$F(\sigma)^{-1} F(\lambda_{j-1}) V_{j-1} = V_j H_{j,j-1}$$

- Updating the matrix $H_{j,j-1}$ according to the linear theory yields

$$\tilde{H}_{j+1,j} = \begin{bmatrix} H_{j,j-1} & k_j \\ 0 & \|r_\perp\| \end{bmatrix},$$

where $k_j = V_j^H r_j$, $r_j = F(\lambda_j) v_j$, and $r_\perp = r_j - V_j V_j^H v_j$.

- Use Lagrangian interpolation to satisfy next Arnoldi relation via

$$G(\lambda_j) \approx \frac{\lambda_j - \sigma}{\lambda_{j-1} - \sigma} G(\lambda_{j-1}) - \frac{\lambda_j - \lambda_{j-1}}{\lambda_{j-1} - \sigma} I = \frac{1}{1-\theta} G(\lambda_{j-1}) - \frac{\theta}{1-\theta} I,$$

where $G(\lambda) := F(\sigma)^{-1} F(\lambda)$, and updates H according to

$$H_{j+1,j} = \begin{bmatrix} \frac{1}{1-\theta} H_{j,j-1} - \frac{\theta}{1-\theta} I_{j,j-1} & k_j \\ 0 & \|r_\perp\| \end{bmatrix}.$$

Discussion

- This first version of the rational Krylov method is not very efficient.
- Ruhe 2000 suggested to modify λ and H in an inner iteration until the residual $r = F(\sigma)^{-1}F(\lambda)V_j s$ is enforced to be orthogonal to V_j
- Expand the search space only after the inner iteration has converged

Rational Krylov algorithm

1: $V = [v_1]$ with $\|v_1\| = 1$, init. λ, σ ; $j = 1$, $h_j = 0_j$; $s = e_j$; $x = v_j$;
2: compute $r = F(\sigma)^{-1}F(\lambda)x$ and $k_j = V_j^H r$
3: **while** $\|k_j\| >$ResTol **do**
4: orthogonalize $r = r - V_j^H k_j$
5: set $h_j = h_j + k_j s_j^{-1}$
6: $\theta =$ min eig $H_{j,j}$ with corresponding eigenvector s
7: $x = V_j s$
8: update $\lambda = \lambda + \frac{\theta}{1-\theta}(\lambda - \sigma)$
9: update $H_{j,j} = \frac{1}{1-\theta}H_{j,j} - \frac{1}{1-\theta}I$
10: compute $r = F(\sigma)^{-1}F(\lambda)x$ and $k_j = V_j^H r$
11: **end while**
12: compute $h_{j+1,j} = \|r\|$
13: **if** $|h_{j+1,j}s_j| >$EigTol **then**
14: $v_{j+1} = r/h_{j+1,j}$; $j = j + 1$; GOTO 2:
15: **end if**
16: Accept eigenvalue $\lambda_i = \lambda$ and eigenvector $x_i = x$
17: If more eigenvalues wanted, choose next θ and s, and GOTO 8:

Variation of Rat. Krylov

start with initial vector $V = [v_1]$ with $\|v_1\| = 1$, initial λ and σ
for $j = 1, 2, \ldots$ until convergence **do**
    solve projected eigenproblem $V^H F(\sigma)^{-1} F(\lambda) V s = 0$ for (λ, s)
    by inner iteration
    compute Ritz vector $x = Vs$ and residual $r = F(\sigma)^{-1} F(\lambda) x$
    orthogonalize $r = r - VV^H r$
    expand searchspace $V = [V\ ,\ r/\|r\|]$
end for

Vibrations of a fluid–solid structure

- Free vibrations of a tube bundle immersed in a slightly compressible fluid.
- Discretizing by finite elements one obtains

$$F(\lambda)x := -Kx + \lambda Mx + \sum_{j=1}^{k} \frac{\lambda}{\sigma_j - \lambda} C_j x = 0,$$

where K, M, and C_j are symmetric matrices, K and C_j are positive semidefinite, M is positive definite, and $0 =: \sigma_0 < \sigma_1 < \cdots < \sigma_k < \sigma_{k+1} := \infty$ are positive.

- In each of the intervals (σ_j, σ_{j+1}), $j = 0, \ldots, k$.
- This problem satisfies the min-max characterization.
- Consider $n = 22654$ with one pole $\sigma_1 = 1$ which has 11 eigenvalues $\lambda_1 \leq \cdots \leq \lambda_{11}$ in the interval $J_1 = (0, 1)$ and a large number of eigenvalues greater than 1, 10 of which are contained in the interval $(1, 4)$.

Results

Method	Iter.	LU fact.	CPU [s]	nlin.sol. [s]
Arnoldi	34	2	14.93	0.13
Jacobi–Davidson	37	3	112.84	0.15
rational Krylov	40	2	70.80	0.22
interval $(1, 4)$				
Arnoldi	36	2	17.35	0.17
Jacobi–Davidson	37	5	125.87	0.23

Damped vibrations of a structure

As second example we consider the free vibrations of a finite element model of dimension 10704 for a solid using a viscoelastic constitutive relation to describe the behavior of the material.

Method	Iter.	LU fact.	CPU [s]	nlin.sol. [s]
Arnoldi	144	2	707.0	469.9
Arnoldi, restarted	139	5	199.6	25.0
Jac.–Davids.	111	9	1050.5	161.2
Jac.–Davids, rest.	109	12	914.4	18.9
rational Krylov	147	3	1107.1	465.3
rational Krylov, rest.	147	4	647.8	28.5

Conclusions

- Industrial applications lead to challenging mathematical problems.
- Large scale nonlinear PDE eigenvalue problems within optimization loop.
- The mathematical theory and algorithms are still far from the needs in reality.
- Commercially available codes are not satisfactory.
- Industry is not interested in and does not pay for the analysis, convergence proofs, etc.
- Structure preserving linearization techniques have been derived.
- Homotopy and Newton like method have been developed but the understanding is open.

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Thank you very much
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