

Structure preservation in eigenvalue computation: a challenge and a chance

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Consider eigenvalue problem

$$P(\lambda) \mathbf{x} = \mathbf{0},$$

where

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



Definition

A nonlinear matrix function $P(\lambda)$ is called

- ▷ **T-even (H-even)** if $P(\lambda) = P(-\lambda)^T (P(\lambda) = P(-\lambda)^H)$;
- ▷ **T-palindromic (H-palindromic)** if $P(\lambda) = \operatorname{rev} P(\lambda)^T (P(\lambda) = \operatorname{rev} P(\lambda)^H)$.

In the following we often drop the prefix T and H.



Let

$$J = \left[\begin{array}{cc} 0 & I_n \\ -I_n & 0 \end{array} \right].$$

- ▷ A matrix *H* is called Hamiltonian if $(JH)^H = JH$ and skew-Hamiltonian if $(JH)^H = -JH$.
- Hamiltonian matrices from a Lie algebra, skew-Hamiltonian matrices form a Jordan algebra.
- ▷ A matrix *S* is called symplectic if $S^H J S = J$.
- ▷ Symplectic matrices form a Lie group.

Proposition

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 , $-\lambda$.

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

Even matrix polynomials have Hamiltonian spectrum, they naturally generalize Hamiltonian problems $\lambda I + H$, where H is Hamiltonian.

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Properties of palindromic matrix functions.

Proposition

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 , $1/\lambda$.

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

Palindromic matrix polynomials have symplectic spectrum, they naturally generalize symplectic problems $\lambda I + S$, where S is a symplectic matrix.

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Definition

Let $P(\lambda)$ be a matrix polynomial of degree *k*. Then the Cayley transformation of $P(\lambda)$ with pole at -1 is the matrix polynomial

$$\mathcal{C}_{-1}(\boldsymbol{P})(\mu) := (\mu+1)^k \boldsymbol{P}\left(rac{\mu-1}{\mu+1}
ight)$$

- The Cayley transformation creates a one-to-one map between palindromic and even polynomials (as it does between symplectic and Hamiltonian matrices).
- ▷ For the theory we only need to treat one structure, the results for the other follow automatically.
- ▷ For numerical methods one has to be careful.





We will not discuss two other important structured classes.

▷ Real or complex symmetric nonlinear evp's. P(λ) = P(λ)^T
▷ Hermitian or real symmetric P(λ)^H = P(λ̄).
▷ ...

For more on these problems see work by Voss '03, Schreiber '08





Introduction Applications

Linearization theory

Trimmed linearization

Numerical methods for structured pencils

Structured restarted Arnoldi for large even evp's
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Excitation of rails and trains

Hilliges 04, Hilliges/Mehl/M. 04. Eigenvalues of $P(\lambda) = \lambda^2 A + \lambda B + A^T$, $B = B^T$, A low rank. Complex T-palindromic problem.





3D elastic field near crack

Apel/M./Watkins 02 $P(\lambda) = \lambda^2 M(\alpha) + \lambda D(\alpha) - K(\alpha)$, $M = M^T > 0$, $K = K^T \ge 0$, $D = -D^T$ for $\alpha \in [a, b]$ real even problem

Example: Crack in 3D Domain Ω





Minimize
$$\sum_{j=0}^{\infty} \left(x_j^H Q x_j + x_j^H Y u_j + u_j^H Y^H x_j + u_j^H R u_j \right)$$

subject to the *k*th-order discrete-time control system

$$\sum_{i=0}^k M_i x_{j+i+1-k} = B u_j, \quad j=0,1,\ldots,$$

with starting values $x_0, x_{-1}, \ldots, x_{1-k} \in \mathbb{R}^n$ and coefficients $Q = Q^H \in \mathbb{R}^{n,n}, Y \in \mathbb{R}^{n,m}, R = R^H \in \mathbb{R}^{m,m}, M_i \in \mathbb{R}^{n,n}, B \in \mathbb{R}^{n,m}.$ Classical case: $\hat{R} = \begin{bmatrix} Q & Y \\ Y^H & R \end{bmatrix}$ positive definite, $M_k = I.$ H_{∞} control: \hat{R} indef. or singular, descriptor case: M_k singular.



Optimality system

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Discrete bvp with palindromic matrix polynomial

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Even matrix Polynomials.

- Passivation of linear control systems arising from model reduced semidisc. Maxwell equations Freund/Jarre '02, Brüll '08
- Optimal control of higher order DAEs M./Watkins '02
- ▷ Gyroscopic systems Lancaster '04, Hwang/Lin/M. '03.
- Optimal Waveguide Design, Schmidt/Friese/Zschiedrich/Deuflhard '03.
- \triangleright H_{∞} control for descriptor Benner/Byers/M./Xu '04.

While Hamiltonian matrices cover only special cases, even matrix polynomials cover all the cases.



Palindromic Matrix Polynomials.

- ▷ Periodic surface acoustic wave filters Zaglmeyer 02.
- Computation of the Crawford number Higham/Tisseur/Van Dooren 02.
- ▷ H_∞ control for discrete time descriptor systems Losse/M./Poppe/Reis '08
- Passivation of discrete linear control systems arising from model reduced fully Maxwell equations Brüll '08

While symplectic matrices cover only special cases, palindromic matrix polynomials cover all the cases.





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Definition

For a matrix polynomial $P(\lambda)$ of degree k, a matrix pencil $L(\lambda) = (\lambda \mathcal{E} + \mathcal{A})$ is called linearization of $P(\lambda)$, if there exist nonsingular unimodular matrices (i.e., of constant nonzero determinant) $S(\lambda)$, $T(\lambda)$ such that

$$S(\lambda)L(\lambda)T(\lambda) = \operatorname{diag}(P(\lambda), I_{(n-1)k}).$$

A linearization is called strong if also revL is a linearization of revP.



Example The quadratic even eigenvalue problem

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

with $M = M^T$, $K = K^T$, $G = -G^T$ has Hamiltonian spectrum but 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 preserve this structure.

- Numerical methods destroy eigenvalue symmetries in finite arithmetic !
- Perturbation theory requires structured perturbations for stability near imaginary axis. Ran/Rodman 1988.

> Can we find structure preserving linearizations.



Vector space of linearizations

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

Definition (Mackey²/Mehl/M. '06.)

For a given $n \times n$ matrix polynomial $P(\lambda)$ of degree *k* define the sets:

$$\begin{aligned} \mathcal{V}_{P} &= \{ \mathbf{v} \otimes \mathbf{P}(\lambda) : \mathbf{v} \in \mathbb{F}^{k} \}, \ \mathbf{v} \text{ is called right ansatz vector}, \\ \mathcal{W}_{P} &= \{ \mathbf{w}^{T} \otimes \mathbf{P}(\lambda) : \mathbf{w} \in \mathbb{F}^{k} \}, \ \mathbf{w} \text{ is called left ansatz vector}, \\ \mathbb{L}_{1}(P) &= \left\{ L(\lambda) = \lambda \mathcal{E} + \mathcal{A} : \mathcal{E}, \mathcal{A} \in \mathbb{F}^{kn \times kn}, L(\lambda) \cdot (\Lambda \otimes I_{n}) \in \mathcal{V}_{P} \right\}, \\ \mathbb{L}_{2}(P) &= \left\{ L(\lambda) = \lambda \mathcal{E} + \mathcal{A} : \mathcal{E}, \mathcal{A} \in \mathbb{F}^{kn \times kn}, \left(\Lambda^{T} \otimes I_{n} \right) \cdot L(\lambda) \in \mathcal{W}_{P} \right\} \\ \mathbb{D}\mathbb{L}(P) &= \mathbb{L}_{1}(P) \cap \mathbb{L}_{2}(P) . \end{aligned}$$

Are there structured linearizations in these classes?



Lemma

Consider an $n \times n$ even matrix polynomial $P(\lambda)$ of degree k. For an ansatz vector $\mathbf{v} = (\mathbf{v}_1, \dots, \mathbf{v}_k)^T \in \mathbb{F}^k$ the linearization $L(\lambda) = \lambda X + Y \in \mathbb{DL}(P)$ is even, i.e. $X = X^T$ and $Y = -Y^T$, (or $X = X^H$ and $Y = -Y^H$,) if and only if the *v*-polynomial

$$\rho(\mathbf{v}; \mathbf{x}) := \mathbf{v}_1 \mathbf{x}^{k-1} + \ldots + \mathbf{v}_{k-1} \mathbf{x} + \mathbf{v}_k$$

is even.

What are appropriate even polynomials p(v; x).



If *P* is real, quadratic, even and has ev ∞ , then there is no even linearization.

Example: Let

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

be even, i.e. $M = M^T$, $D = -D^T$, $K = K^T$.

If *M* is singular, then the even linear pencil (obtained with $v = e_2$)

$$\lambda \left[\begin{array}{cc} \mathbf{0} & -\mathbf{M} \\ \mathbf{M} & \mathbf{G} \end{array} \right] + \left[\begin{array}{cc} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{K} \end{array} \right]$$

is not a linearization, since $L(\lambda)$ is not regular.

We can alternatively look at odd problems, then the ev. 0 is 'bad'.



Lemma (Mackey/Mackey/Mehl/M. '06)

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

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

What are appropriate palindromic polynomials p(v; x).



Example: For the palindromic polynomial

$$P(\lambda)y = (\lambda^2 A + \lambda B + A^T)y = 0, \ B = B^T$$

all palindromic vectors have the form $v = [\alpha, \alpha]^T$, $\alpha \neq 0$ leads to a palindromic pencil

$$\kappa Z^{T} + Z, \ Z = \begin{bmatrix} A & B - A^{T} \\ A & A \end{bmatrix}$$

This is a linearization iff if -1 is not an eigenvalue of $P(\lambda)$. We can alternatively look at anti-palindromic linearizations, then the ev. 1 is 'bad'.





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To get good numerical results it is essential to deflate 'bad' ev's from the polynomial problem.

- \triangleright Compute appropriate (structured) staircase form associated with the eigenvalues 1, -1, 0, ∞ and the singular part directly for matrix polynomial.
- ▷ Remove parts associated with eigenvalues 1, -1, 0, ∞ and singular parts. This can (at least in principle) be done exactly.
- Perform (structured) linearization on the resulting 'trimmed' matrix polynomial.
- ▷ 'Near bad' eigenvalues, however, lead to ill-conditioning.

Theorem (Byers/M./Xu 07)

Let $A_i \in \mathbb{C}^{m,n}$ i = 0, ..., k. Then, the tuple $(A_k, ..., A_0)$ is unitarily equivalent to a matrix tuple $(\hat{A}_k, \ldots, \hat{A}_0) = (UA_kV, \ldots, UA_0V)$, all terms \hat{A}_i , i = 0, ..., k have form A A A A $A_1^{(i)}$ $A_0^{(i)}$ 0 $\tilde{A}_{1}^{(i)}$ 0



- ▷ Each of the blocks $A_j^{(i)}$ i = 0, ..., k, j = 1, ..., I either has the form $\begin{bmatrix} \Sigma & 0 \end{bmatrix}$ or $\begin{bmatrix} 0 & 0 \end{bmatrix}$,
- ▷ Each of the blocks $\tilde{A}_{j}^{(i)}$ i = 1, ..., k, j = 1, ..., l either has the form $\begin{bmatrix} \Sigma \\ 0 \end{bmatrix}$ or $\begin{bmatrix} 0 \\ 0 \end{bmatrix}$.
- ▷ For each *j* only of the $A_i^{(i)}$ and $\tilde{A}_i^{(i)}$ is nonzero.
- ▷ In the tuple of middle blocks $(A_0^{(k)}, \ldots, A_0^{(k)})$ (essentially) no k of the coefficients have a common nullspace.



- Structured staircase forms for even and palindromic polynomials and pencils under congruence Byers/M./Xu '07.
- There exist exceptional cases where the 'bad' ev's cannot be removed.
- In many cases exactly 'bad' eigenvalues can be deflated ahead in a structure preserving way. This leads to 'trimmed linearizations'.
- $\triangleright\,$ In all the industrial examples the ev's 0 and $\infty,\pm 1$ can be removed without much computational effort, just using the structure of the model.
- ▷ Singular parts can be removed altogether.



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.



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

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





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- Structure preserving QR/QZ like methods for even pencils Benner/M./Xu '97, '98, Chu/Liu/M. '04, Byers/Kressner '07
- Structure preserving Arnoldi method and JD methods for even pencils M./Watkins '01, Apel/M./Watkins '02, Hwang/Lin/Mehrmann '03
- Palindromic Jabobi and Laub trick Mackey², Mehl, M. '07;
- Palindromic QR/QZ algorithm and URV algorithm Dissertation Schröder 07;
- Recursive doubling Chu/Lin/Wang/Wu '05

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Introduction Applications Linearization theory Trimmed linearization Numerical methods for structured pencils Structured restarted Arnoldi for large even evp's Conclusions

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For the even quadratic $P(\lambda) = \lambda^2 M + \lambda G - K$ with $M = M^T > 0, K = K^T > 0, G = -G^T$ we have the even linearization:

$$\lambda \mathbf{N} - \mathbf{W} = \lambda \begin{bmatrix} \mathbf{0} & -\mathbf{M} \\ \mathbf{M} & \mathbf{G} \end{bmatrix} - \begin{bmatrix} -\mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{K} \end{bmatrix}$$

with $N = -N^T$, $W = W^T$.

This can be transformed to a Hamiltonian matrix.

- \triangleright $N = Z_1 Z_2$, $Z_2^T J = \pm J Z_1$, sparse J-Cholesky factorization.
- ▷ Transform to $\lambda I H = \lambda I Z_1^{-1} W Z_2^{-1}$, where $H = Z_1^{-1} W Z_2^{-1}$ is Hamiltonian.

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$$H = Z_1^{-1}WZ_2^{-1}$$

$$= \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -K \\ M^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix}$$

$$H^{-1} = \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & M \\ (-K)^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix}$$

Multiplication with H or H^{-1} only needs solves with mass matrix M or stiffness matrix K, respectively. Note that 'bad' eigenvalues are removed.



Form Krylov basis

$$[q_1, Aq_1, A^2q_1, \ldots, A^\ell q_1]$$

and orthogonalize vectors. Ordinary Arnoldi process

$$q_{j+1} = Aq_j - \sum_{i=1}^j q_i h_{ij}.$$

With $Q_\ell = [q_1, q_2, \dots, q_\ell]$ we have

$$m{A}m{Q}_\ell = m{Q}_\ellm{H}_\ell + m{f}_\ellm{e}_\ell^T$$

and use eigenvalues of the Hessenberg matrix H_{ℓ} as approximations to eigenvalues of A.



- Loss of orthogonality in the process leads to spurious eigenvalues, i.e. the same eigenvalues converge again and again.
- To avoid this, we can reorthogonalize or restart. But this expensive, so to make this feasible: Implicit restart. ARPACK, Lehoucq, Sorensen Yang 1998.
- ▷ Typically we get convergence of exterior eigenvalues.
- Only in the symmetric case a complete convergence theory is avaliable.
- ▷ To get interior eigenvalues we can use shift-and-invert
- Arnoldi does not respect the structure.



Start: Build a length / Arnoldi process.

$$m{A}m{Q}_\ell = m{Q}_\ellm{H}_\ell + m{f}_\ellm{e}_\ell^T$$

For $i = 1, 2, \dots$ until satisfied:

- 1. Compute eigenvalues of H_{ℓ} and split them into a wanted set $\lambda_1, \ldots, \lambda_k$ and an unwanted set $\lambda_{k+1}, \ldots, \lambda_{\ell}$.
- 2. Perform $p = \ell k$ steps of the QR-iteration with the unwanted eigenvalues as shifts and obtain $H_{\ell}V_{\ell} = V_{\ell}\tilde{H}_{\ell}$.
- 3. Restart: Postmultiply by the matrix V_k consisting of the *k* leading columns of V_{ℓ} .

$$AQ_{\ell}V_{k} = Q_{\ell}V_{k}\tilde{H}_{k} + \tilde{f}_{k}e_{k}^{T},$$

where \tilde{H}_k is the leading $k \times k$ principal submatrix of \tilde{H}_ℓ .

4. Set $Q_k = Q_\ell V_k$ and extend Arnoldi factorization to length ℓ .



To obtain interior eigenvalues we use shift-and-invert, i.e., we apply the implicitly restarted Arnoldi to a rational function of the matrix.

Goals:

- Pick shift point near the region where the desired eigenvalues are.
- Use a rational transformation that retains the eigenvalue symmetry.
- ▷ Transformation must be cheaply computable.



- Hamiltonian
- skew-Hamiltonian

$$H^{-2}$$

$$(H - \tau I)^{-1}(H + \tau I)^{-1}$$

$$(H - \tau I)^{-1}(H + \tau I)^{-1}(H - \overline{\tau} I)^{-1}(H + \overline{\tau} I)^{-1}$$

 H^{-1}

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symplectic

$$(\boldsymbol{H} - \tau \boldsymbol{I})^{-1}(\boldsymbol{H} + \tau \boldsymbol{I})$$
$$(\boldsymbol{H} - \tau \boldsymbol{I})^{-1}(\boldsymbol{H} + \overline{\tau} \boldsymbol{I})(\boldsymbol{H} - \overline{\tau} \boldsymbol{I})^{-1}(\boldsymbol{H} + \tau \boldsymbol{I})$$

 $\tau =$ target shift.

Three different structures, three different methods.



$$W = (H - \tau I)^{-1} (H + \overline{\tau} I)^{-1} (H - \overline{\tau} I)^{-1} (H + \tau I)^{-1}$$

Each factor has the form

$$(H - \tau I)^{-1} = \begin{bmatrix} I & \frac{1}{2}G + \tau M \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -M \\ Q(\tau)^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & \frac{1}{2}G + \tau M \\ 0 & I \end{bmatrix}$$

$$\triangleright \ \mathbf{Q}(\tau) = \tau^2 \mathbf{M} + \tau \mathbf{G} + \mathbf{K}$$

- $\triangleright Q(\tau) = P_q L_q U_q$ (sparse *LU* decomposition)
- ▷ One decomposition for all four factors.

🕸 Skew-Hamiltonian Arnoldi Process SHIRA

Isotropic Arnoldi process

$$ilde{q}_{j+1} = \mathcal{W} q_j - \sum_{i=1}^j q_i h_{ij} - \sum_{i=1}^j J q_i t_{ij}$$

- ▷ produces *isotropic* subspaces: Jq_1, \ldots, Jq_k are orthogonal to q_1, \ldots, q_k .
- ▷ Theory $t_{ij} = 0$. Practice $t_{ij} = \epsilon$ (roundoff)
- Enforcement of isotropy is crucial.
- ▷ Consequence: get each eigenvalue only once.



Input: *H* and
$$\tau = \alpha$$
 or $\tau = i\alpha$, $\alpha \in \mathbb{R}$.

Output: Approx. inv. subspace of *H* ass. with *p* ev's near τ .

- ▷ Generate Arnoldi vectors $Q_k = [q_1, ..., q_k]$ and upper Hessenberg $H_k \in \mathbb{R}^{k \times k}$ such that $(H^2 - \tau^2 I)^{-1}Q_k = Q_k H_k$. Compute $\Omega_k = H_k^{-1} + \lambda_0^2 I$.
- ▷ Compute the real Schur decomposition $\Omega_k = U_k T_k U_k^T$.
- ▷ Reorder the *p* desired stable eigenvalues of T_k to the top of T_k , i.e., $T_k = V_k \begin{bmatrix} T_{11} & T_{12} \\ 0 & T_{22} \end{bmatrix} V_k^T$, where $T_{11} \in \mathbb{R}^{p \times p}$ has desired eigenvalues.

$$\triangleright \text{ Set } \tilde{Q}_p := Q_k U_k V_k \left[\begin{array}{c} I_p \\ 0 \end{array} \right].$$

- ▷ Compute the unique positive square root $T_{11}^{1/2}$ of T_{11} .
- ▷ Compute the stable invariant subspace $V_{\rho} = H\tilde{Q}_{\rho} \tilde{Q}_{\rho} T_{11}^{1/2}$.



Numerical Results: Fichera Corner

Discretized Problem n = 2223, asking for 6 ev's in right half-pl.

- $\lambda_1 = 0.96269644895$
- $\lambda_2 = 0.98250961158 + 0.00066849814i$
- $\lambda_3 = 0.98250961158 0.00066849814i$
- $\lambda_4 = 1.35421843051$
- $\lambda_5 = 1.39562564903$
- $\lambda_6 = 1.49830518846.$

	flops (10 ⁷)	
τ	SHIRA	unstructured
0	32.6	140.1
0.3	32.6	79.6
0.6	25.7	69.8
0.9	23.0	50.7
1.2	17.5	31.5



Computing times

Crack example: CPU in *s* for 15 ev's in [0,2), $h = \pi/120$; $\tau = 0$, solid line: SHIRA, dashed line: IRA with $(H - \tau I)^{-1}$;





Example: Fichera Corner

Eigenvalues for various material parameters





Results of SHIRA for Crack problem

Ev's with real part in (0.1,2.1). Dashed: nonreal eigenvalues. Triple ev's $\alpha = 0$ and $\alpha = 1$, 3 simple real ev's.







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- Palindromic and even polynomial eigenvalue problems are important in many applications.
- Structured linearization methods are available.
- ▷ Structured staircase forms are available.
- ▷ New trimmed linearization techniques are available.
- Structure preserving numerical methods for small even and palindromic pencils have been constructed.
- Structure preserving numerical methods for large sparse even and palindromic pencils have been constructed (provided we can still factor).

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Thank you very much for your attention.

information, papers, codes etc

http://www.math.tu-berlin.de/~mehrmann



T. Apel, V. Mehrmann and D. Watkins, *Structured eigenvalue methods for the computation of corner singularities in 3D anisotropic elastic structures.* COMP. METH. APPL. MECH. AND ENG., 2002.

R. Byers, V. Mehrmann and H. Xu. A structured staircase algorithm for skew-symmetric/symmetric pencils, ETNA, 2007. R. Byers, V. Mehrmann and H. Xu. Staircase forms and trimmed linearization for structured matrix polynomials. PREPRINT, MATHEON, url: http://www.matheon.de/ 2007. D.S. Mackey, N. Mackey, C. Mehl and V. Mehrmann. Vector spaces of linearizations for matrix polynomials, SIMAX 2007. D.S. Mackey, N. Mackey, C. Mehl and V. Mehrmann. Structured Polvnomial Eigenvalue Problems: Good Vibrations from Good Linearizations, SIMAX 2007.

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V. Mehrmann and H. Voss: *Nonlinear Eigenvalue Problems: A Challenge for Modern Eigenvalue Methods.* GAMM Mitteilungen, 2005.

C. Schröder: *A QR-like algorithm for the palindromic eigenvalue problem*. PREPRINT, MATHEON, *url: http://www.matheon.de/*, 2007.

C. Schröder: URV decomposition based structured methods for palindromic and even eigenvalue problems. PREPRINT,

MATHEON, url: http://www.matheon.de/, 2007.

C. Schröder: Palindromic and even eigenvalue problems.

Analysis and numerical methods. Dissertation, TU Berlin, 2008.

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