Rational Krylov Methods for the Hamiltonian Eigenvalue Problem

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Fakultät für Mathematik

TECHNISCHE UNIVERSITÄT CHEMNITZ

Outline

Hamiltonian Matrices

$$H = \begin{bmatrix} A & B \\ C & -A^T \end{bmatrix}$$

$$B^T = B \in \mathbb{R}^{n\times n}, C^T = C \in \mathbb{R}^{n\times n}, A \in \mathbb{R}^{n\times n}$$

Alternatively:

$$H^T = JHJ$$

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$$

I is the $n \times n$ identity matrix.

$$J^{-1} = J^T = -J$$

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Spectral Structure

Let x be a right eigenvector of H corresponding to eigenvalue λ

$$Hx = \lambda x$$

$$JHx = \lambda Jx$$

$$JHJJ^T x = -\lambda J^T x$$

$$H^T(J^T x) = -\lambda(J^T x)$$

$J^T x$ is a left eigenvector of H corresponding to eigenvalue $-\lambda$

- spectrum symmetric with respect to imaginary axis
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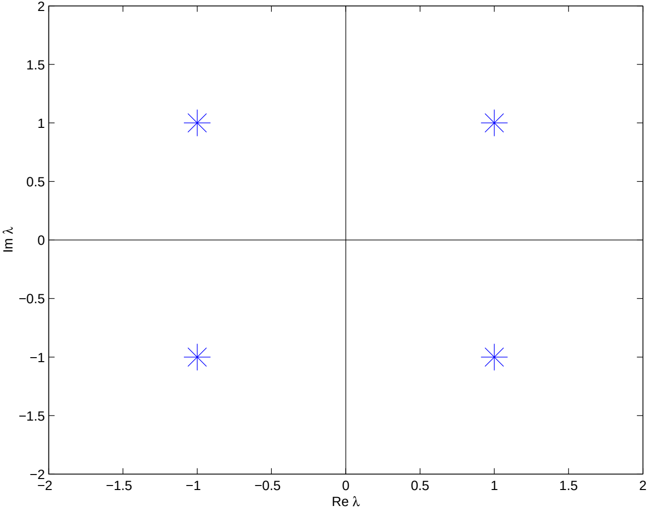
Eigenvalue Quadruples



- considered matrices are large and sparse
- cannot compute all eigenvalues and eigenvectors
- want just a few of them

$\Longrightarrow$ Krylov Subspace Methods (Lanczos / Arnoldi)

- recursive scheme to compute expanding Krylov subspaces

$$HU_j = U_j T_j + u_{j+1}\beta_j e_j^T$$

- U_j's columns span the Krylov subspace
- Rayleigh quotient $T_j = U_j^T H U_j$ is the projection of H onto this Krylov subspace
- T_j's eigenvalues approximate H's eigenvalues

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Structure Preservation

- spectrum of Rayleigh quotient is unstructured in general
- want to preserve eigenvalue pairings

$$S \in \mathbb{R}^{2n \times 2k} \text{ symplectic } \iff S^T J S = J$$

- if U_j is symplectic, the Rayleigh quotient will inherit the Hamiltonian structure

$\Longrightarrow$ Hamiltonian Lanczos Process
(Freund & Mehrmann, 1994; Benner & Fassbender, 1997; Ferng & Liu & Wang, 1997)

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Spectral Transformation

- Krylov subspace methods tend to approximate extremal eigenvalues first
- getting interior eigenvalues may be considerably more work

- idea: apply the method to $(H - \mu I)^{-1}$ instead of H
- eigenvalues λ_i of $H \implies$ eigenvalues $\frac{1}{\lambda_i - \mu}$ of $(H - \mu I)^{-1}$
- same eigenvectors
- eigenvalues near the shift μ are mapped to eigenvalues of large modulus

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Rational Krylov Method

- shift-and-invert Lanczos / Arnoldi throws away the Krylov basis once the eigenvalues near the shift have converged
- waste of information
- Rational Krylov Method (Axel Ruhe, 1992) allows changes of shift during runtime
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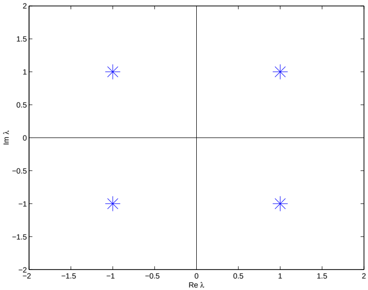
Goals

We want to construct a method capable of both

- preserving the Hamiltonian spectral symmetry and
- allowing runtime changes of shift.

Hamiltonian Spectral Transformation



- conventional way of shifting destroys Hamiltonian spectral symmetry
- shifts should also occur in pairs $\mu, -\mu$
- Mehrmann & Watkins, 2001 proposed to use the composite shift operator $(H - \mu I)^{-1}(H + \mu I)^{-1}$

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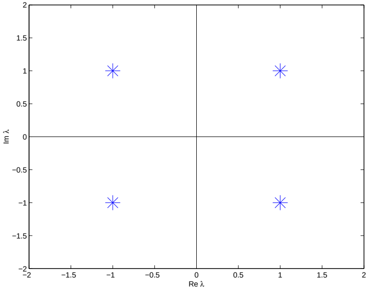

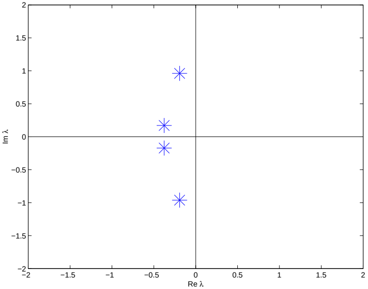

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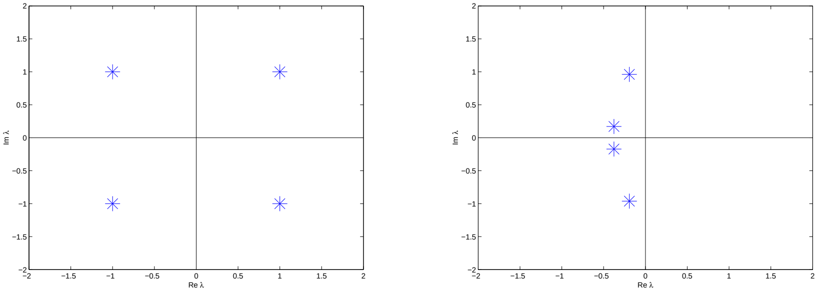

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Skew-Hamiltonian Matrices

- $(H - \mu I)^{-1}(H + \mu I)^{-1}$ has Skew-Hamiltonian structure

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- all eigenvalues have even algebraic and geometric multiplicities
- structure is preserved by symplectic transformations

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Composite Shift Operator

- $(H - \mu I)^{-1}(H + \mu I)^{-1} = (H^2 - \mu^2 I)^{-1}$
- eigenvalue λ of H is transformed to $\frac{1}{\lambda^2 - \mu^2}$
- sign information is lost when squaring
- but it can be restored
- eigenspaces for λ and $-\lambda$ are merged

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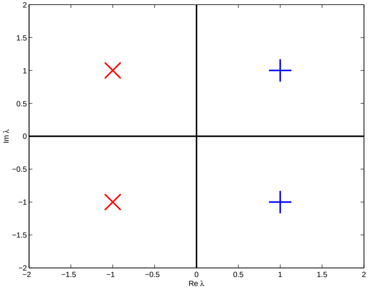

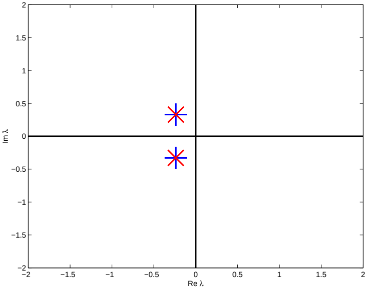

Solution of the Skew-Hamiltonian Problem

- apply the Arnoldi method

$$(H^2 - \mu^2 I)^{-1} U_k = U_k T_k + u_{k+1} t_{k+1,k} e_k^T$$

- U_k spans a Krylov subspace
- $T_k = U_k^T (H^2 - \mu^2 I)^{-1} U_k$ is the corresponding Rayleigh quotient

- it can be shown that $U_k^T J U_k = 0$
- therefore $\left[U_k, J^T U_k\right]$ is orthogonal and symplectic

$$\left[U_k, J^T U_k\right]^T (H^2 - \mu^2 I)^{-1} \left[U_k, J^T U_k\right] = \begin{bmatrix} T_k & * \\ 0 & T_k^T \end{bmatrix}$$

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SHIRA

- in inexact arithmetic $U_k^T J U_k = 0$ has to be enforced

$\Longrightarrow$ SHIRA

- the shift μ is still fixed
- we want to derive a modification of SHIRA that permits changes of shift

$$(H^2 - \mu^2 I)^{-1} U_k = U_k T_k + u_{k+1} t_{k+1,k} e_k^T$$

- split this equation columnwise

$$(H^2 - \mu^2 I)^{-1} u_j = U_{j+1} t_j, \quad j = 1, \ldots, k$$

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Rational Transformation

- we need to transform these equations in order to regain an Arnoldi decomposition

$$(H^2 - \mu_j^2 I)^{-1} u_j = U_{j+1} t_j$$

$$u_j = H^2 U_{j+1} t_j - U_{j+1} t_j \mu_j^2$$

$$H^2 U_{j+1} t_j = u_j + U_{j+1} t_j \mu_j^2$$

$$H^2 U_{j+1} t_j = U_{j+1}(e_j + t_j \mu_j^2)$$

- put identities for $j = 1, \ldots, k$ together; $M_k := \begin{bmatrix} \mu_1 & & \\ & \ddots & \\ & & \mu_k \end{bmatrix}$

$$H^2 U_{k+1} T_{k+1,k} = U_{k+1}(I_{k+1,k} + T_{k+1,k} M_k^2)$$

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- $Q^T (I_{k+1,k} + T_{k+1,k} M_k^2) Z =: \hat{K}_{k+1,k}$ is upper Hessenberg

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- $K_{k+1,k} := \hat{K}_{k+1,k} \hat{T}_k^{-1}$ is upper Hessenberg

$$H^2 V_k = V_{k+1} K_{k+1,k} = V_k K_k + v_{k+1} \beta_k e_k^T$$

- obtained an Arnoldi decomposition of H^2

Rational Transformation III

$$H^2 U_{k+1} Q \hat{T}_{k+1,k} = U_{k+1} Q \hat{K}_{k+1,k}$$

- $U_{k+1} Q =: V_{k+1}$
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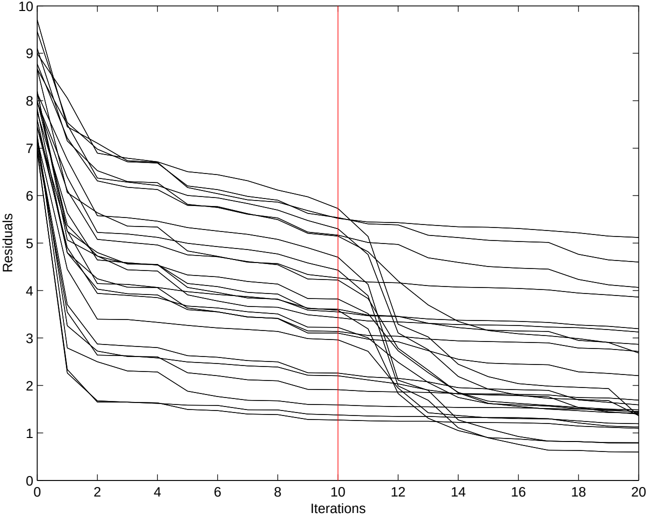
Numerical Results



Summary

- Hamiltonian, Skew-Hamiltonian and symplectic structures
- Hamiltonian and Skew-Hamiltonian spectrum
- Hamiltonian shifting techniques
- transformation of Hamiltonian into Skew-Hamiltonian EVP
- solution of Skew-Hamiltonian problem using Rational Krylov Method

Still Under Development

- method using Hamiltonian structure directly
- avoid the need of eigenvalue reconstruction and other post processing
- will require non-orthogonal symplectic transformations