A Structure-Preserving Method for Large Scale Eigenproblems of Skew-Hamiltonian/Hamiltonian (SHH) Pencils

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New Orleans, July 13, 2005

Goal & Outline

- Usual way:

  SHH pencil $\Rightarrow$ standard Hamiltonian
  $\Rightarrow$ skew-Hamiltonian
  $\Rightarrow$ apply structure-preserving method for eigenvalues

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- Outline
  - Definitions and basics
  - Two applications
  - SHIRA (Mehrmann & Watkins, 2001)
  - SHHA
  - Numerical examples

SHH Pencils

$$\lambda\mathcal{N} - \mathcal{H},$$

skew-Hamiltonian $\mathcal{N} = \begin{bmatrix} F_1 & G_1 \\ H_1 & F_1^* \end{bmatrix}$ with $G_1 = -G_1^*, H_1 = -H_1^*$,

Hamiltonian $\mathcal{H} = \begin{bmatrix} F_2 & G_2 \\ H_2 & -F_2^* \end{bmatrix}$ with $G_2 = G_2^*, H_2 = H_2^*$.

Spectrum symmetry:

- $(\lambda, x, z) \quad \Rightarrow \quad (-\bar{\lambda}, Jz, Jx)$. $J = \begin{bmatrix} & I \\ -I & \end{bmatrix}$.
- $\lambda, -\lambda, \bar{\lambda}, -\bar{\lambda}$ for real SHH.

Two applications

- Passivity checking
  - Linear system $\begin{cases} \dot{x} = Ax + Bu \\ y = Cx + Du \end{cases}$ is passive

    $\Leftrightarrow \mathcal{H} = \begin{bmatrix} A - BR^{-1}D^*C^* & BR^{-1}B^* \\ CS^{-1}C^* & -A^* + CDR^{-1}B^* \end{bmatrix}$ has pure imaginary eigenvalues
  - Compute pure imaginary eigenvalues of a real Hamiltonian matrix
- Complex gyroscopic QEP
  - QEP: $(\lambda^2 M + \lambda j W + K)x = 0$: $M = M^* > 0$, $K = K^* \geq 0$ and $W = -W^*$
  - Linearization:

$$\left(\lambda \begin{bmatrix} M & -W \\ 0 & M \end{bmatrix} - \begin{bmatrix} 0 & -K \\ M & 0 \end{bmatrix}\right) \begin{bmatrix} \lambda x \\ x \end{bmatrix} = 0$$

  - Compute eigenvalues close $a > 0$ of a complex SHH pencil.

Dense Hamiltonian matrices

- All (or half) eigenpairs are to be computed;
- QR algorithm does not preserve structure, computed eigenvalues are not symmetric;
- Structure preserving method
  - orthogonal-symplectic transformation
  - squaring: Hamiltonian $\Rightarrow$ skew-Hamiltonian
  - periodic QR algorithm
  + package: `HAPACK:haeig ...`

Large scale SHH pencils

- Only partial eigenvalues interested: close to τ
- Arnoldi, Lanczos methods: do not preserve structure
- Hamiltonian Lanczos method:
  - structure-preserving
  - only for Hamiltonian eigenvalue, not for a general SHH pencil
  - without shift: Hamiltonian with shift is not Hamiltonian
  - transform to skew-Hamiltonian $\Rightarrow$ apply skew-Hamiltonian Lanczos; or
  - transform to symplectic $\Rightarrow$ apply symplectic Lanczos
- SHIRA: Mehrmann & Watkins, SISC 2001 $\Rightarrow$ next pages

SH(IR)A

Skew-Hamiltonian (Implicit Restart) Arnoldi method.

real SHH pencil $\Rightarrow$ real skew-Hamiltonian:

- $\mathcal{N} = Z_1 Z_2$ with $Z_2^* J = J Z_1$,
- $\lambda\mathcal{N} - \mathcal{H} \Rightarrow \lambda I - \mathcal{W} := \lambda I - Z_1^{-1}\mathcal{H}Z_2^{-1}$
- If τ^2 is real,

$$A = (\mathcal{W} - \tau I)^{-1}(\mathcal{W} + \tau I)^{-1} = Z_2(\mathcal{H} - \tau\mathcal{N})^{-1}\mathcal{N}(\mathcal{H} + \tau\mathcal{N})^{-1}Z_1$$

- otherwise

$$\begin{aligned} A &= (\mathcal{W} - \tau I)^{-1}(\mathcal{W} + \tau I)^{-1}(\mathcal{W} - \bar{\tau} I)^{-1}(\mathcal{W} + \bar{\tau} I)^{-1} \\ &= Z_2(\mathcal{H} - \tau\mathcal{N})^{-1}\mathcal{N}(\mathcal{H} + \tau\mathcal{N})^{-1}\mathcal{N}(\mathcal{H} - \bar{\tau}\mathcal{N})^{-1}\mathcal{N}(\mathcal{H} + \bar{\tau}\mathcal{N})^{-1}Z_1 \end{aligned}$$

A is real skew-Hamiltonian!

SH(IR)A: cont'd

Skew-Hamiltonian (Implicit Restart) Arnoldi (SHIRA) method.

For real skew-Hamiltonian matrix A,

1. Run k steps isotropic Arnoldi procedure

$$AQ = QT + JQS + t_{k+1\,k}q_{k+1}e_k^*,$$

   such that

   - orthogonal: $Q^TQ = I$
   - isotropic: $Q^TJQ = 0$

2. Compute eigenvalue μ of matrix T.

3. Compute approximated eigenvalues λ of original pencil from

$$\lambda^2 - \tau^2 = \frac{1}{\mu} \quad \text{or} \quad (\lambda^2 - \tau^2)(\lambda^2 - \bar{\tau}^2) = \frac{1}{\mu}.$$

SH(IR)A keeps spectrum symmetry! No approximated eigenvectors!

Structure-preserving projection method

Structure-preserving method:

- SHH pencil $\Rightarrow$ SHH pencil?
- any shift τ?
- complex SHH pencil?

A new method: SHHA

Shift-and-invert: $\lambda\mathcal{N} - \mathcal{H} \quad \Rightarrow \quad (\mathcal{H} - \tau\mathcal{N})^{-1}\mathcal{N} - \mu I \equiv A - \mu I.$

Skew-Hamiltonian/Hamiltonian Arnoldi (SHHA) method.

1. Run k steps Arnoldi procedure

$$AQ = QT + t_{k+1\,k}q_{k+1}e_k^*$$

2. Partition $Q = \begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix}$.
3. Oblique projection:

$$\begin{bmatrix} Q_2^* & \\ & Q_1^* \end{bmatrix} (\lambda\mathcal{N} - \mathcal{H}) \begin{bmatrix} Q_1 & \\ & Q_2 \end{bmatrix} \equiv \lambda\mathcal{N}_k - \mathcal{H}_k,$$

4. $\lambda\mathcal{N}_k - \mathcal{H}_k \quad \Rightarrow \quad (\lambda, x, y)$
5. Approximated eigen-triplet: $\left(\lambda, \begin{bmatrix} Q_1 & \\ & Q_2 \end{bmatrix} x, \begin{bmatrix} Q_2 & \\ & Q_1 \end{bmatrix} y\right)$.

Motivation of oblique projection

Theorem For SHH pencil, span $\{Q\}$: right Krylov subspace for shift $\tau \quad \Rightarrow$ span $\{JQ\}$: left Krylov subspace for shift $-\bar{\tau}$

Theorem

$$\text{span}\{Q\} \subseteq \text{span}\left\{\begin{bmatrix} Q_1 & \\ & Q_2 \end{bmatrix}\right\}, \quad \text{and} \quad \text{span}\{JQ\} \subseteq \text{span}\left\{\begin{bmatrix} Q_2 & \\ & Q_1 \end{bmatrix}\right\}.$$

Related work:

- Bai and Su, SIMAX 2005, SISC 2005
- Freund, ICCAD 2004
- Su, Wang, Zeng, Bai, ICCAD 2004
- Chahlaoui, Gallivan, Vandendorpe, and van Dooren, Oberwolfach 2005

Pure imaginary shift τ

When τ pure imaginary:

$\Rightarrow$ $\tau = -\bar{\tau}$,

$\Rightarrow$ span $\{Q\}$: right Krylov subspace, span $\{JQ\}$: left Krylov subspace, same shift.

$\Rightarrow$ twice convergence rate of eigenvalues!

Deflation

When Q_1 or Q_2 is rank deficient:

- $\mathcal{N}_k$ would be singular, reduced-order SHH could be not a regular pencil.
- Important:

$$\operatorname{span}\{Q\} \subseteq \operatorname{span}\left\{\begin{bmatrix} \widehat{Q}_1 & \\ & \widehat{Q}_2 \end{bmatrix}\right\}.$$

- Solution: find $\widehat{Q}_1$ and $\widehat{Q}_2$ of same number of columns such that

$$\operatorname{span}\{Q_1\} \subseteq \operatorname{span}\{\widehat{Q}_1\}, \quad \operatorname{span}\{Q_2\} \subseteq \operatorname{span}\{\widehat{Q}_2\},$$

- Obliquely project with $\begin{bmatrix} \widehat{Q}_1 & \\ & \widehat{Q}_2 \end{bmatrix}$ and $\begin{bmatrix} \widehat{Q}_2 & \\ & \widehat{Q}_1 \end{bmatrix}$.

Reduce to a standard Hamiltonian eigenvalue problem

When $\mathcal{N} = I$:

- get Q_1 and Q_2
- biorthogonalize Q_1 and Q_2 such that $Q_2^* Q_1 = I$;
- obliquely project with Q_1 and Q_2;
- $\mathcal{H} - \lambda I \quad \Rightarrow \quad \mathcal{H}_k - \lambda I$.

Real arithmetic for real pencil with complex shift

real SHH pencil $\Rightarrow$ real reduced-order SHH pencil?

- construct Krylov subspace with

$$Re(\mathcal{H} - \tau\mathcal{N})^{-1}\mathcal{N} \ \text{ or } \ Im(\mathcal{H} - \tau\mathcal{N})^{-1}\mathcal{N}$$

  – Parlett and Saad (1987); ARPARK;

- construct Krylov subspace with

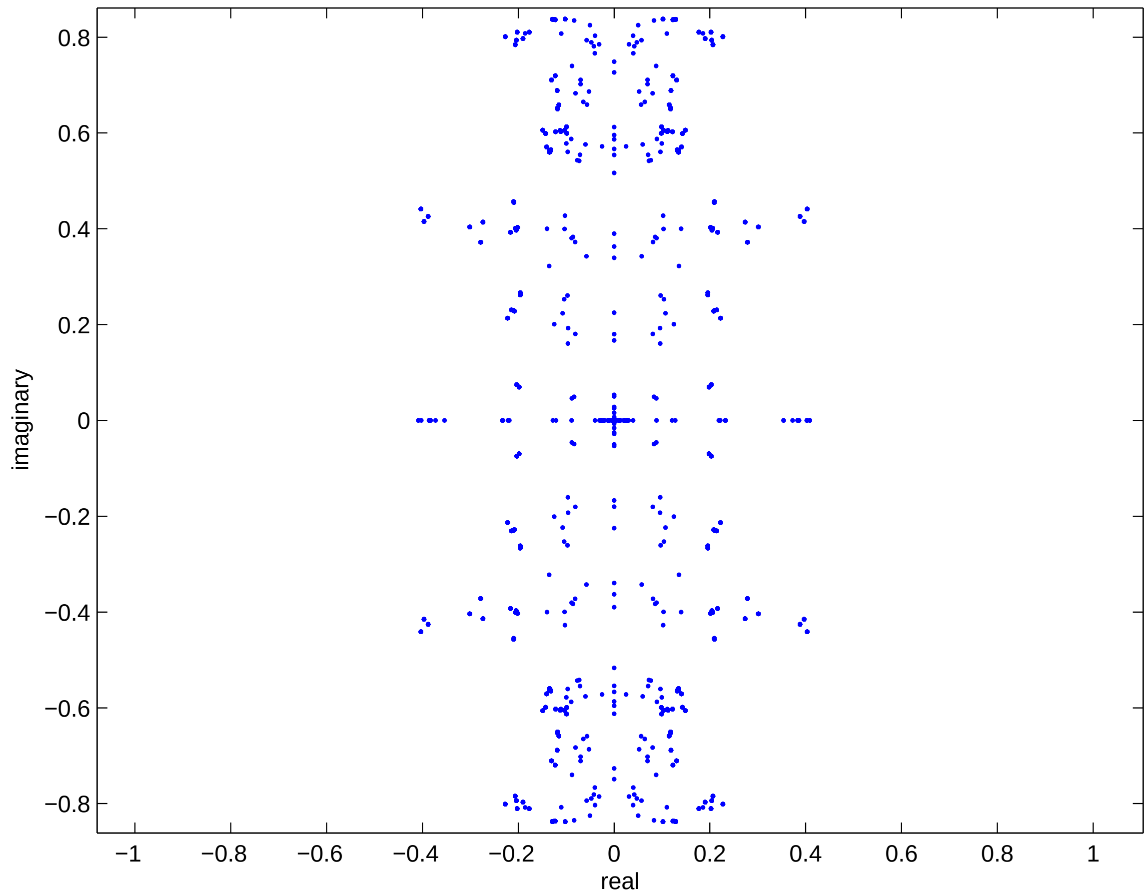
$$(\mathcal{H} - \tau\mathcal{N})^{-1}\mathcal{N}(\mathcal{H} - \bar{\tau}\mathcal{N})^{-1}\mathcal{N}$$

  – for pure imaginary τ, it does not work
  – for complex τ, some potential bugs

Not completely solved yet even for unstructured algorithm (e.g. Arnoldi) for unstructured eigenvalue problem. Remains OPEN!

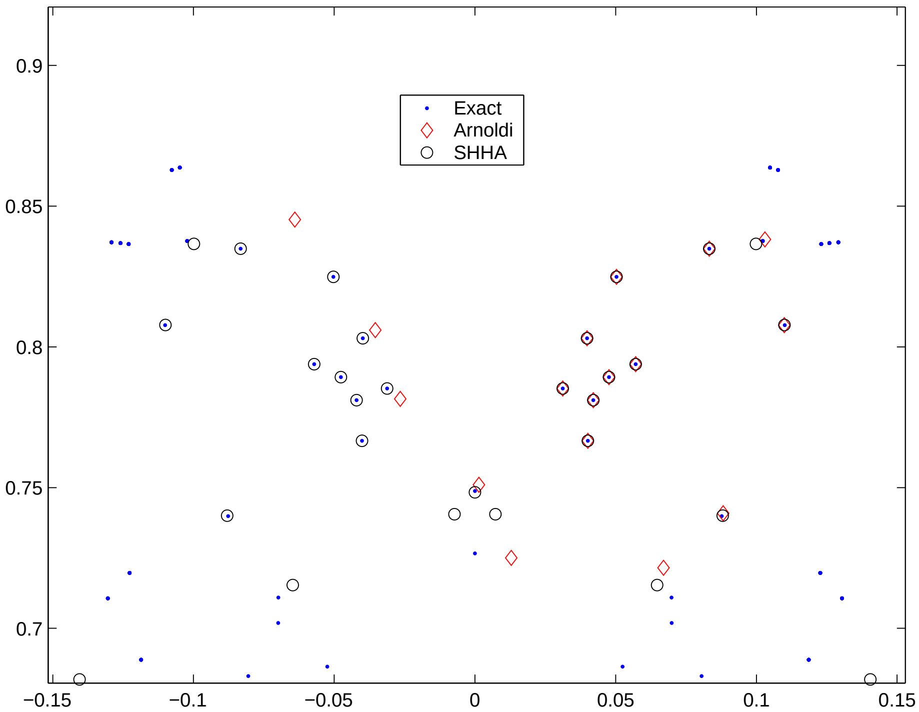
Numerical example 1

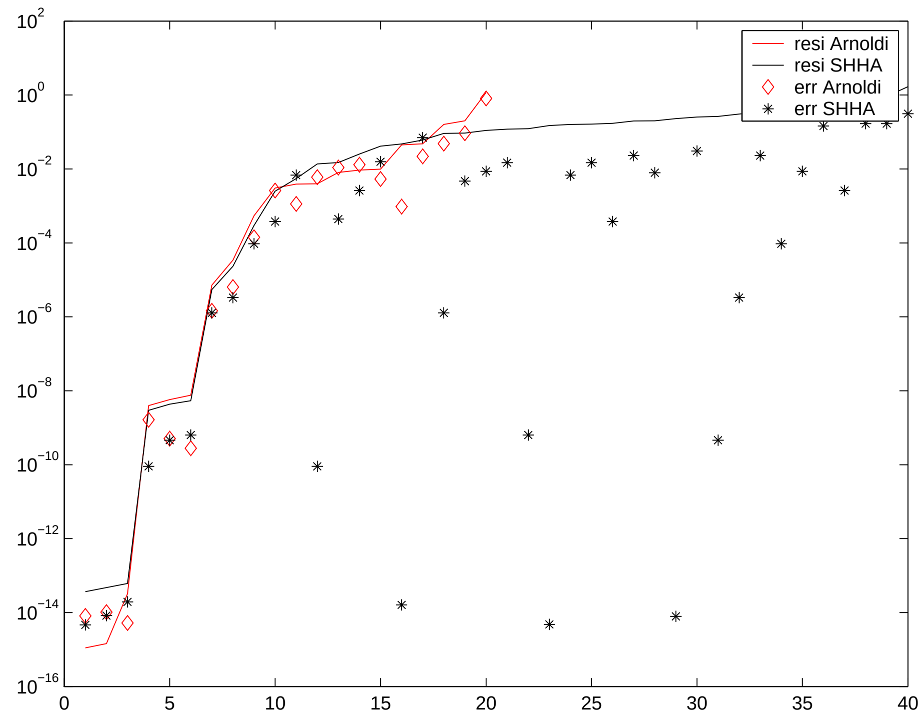
- Passivity checking
- 1988 state variables, 12 inputs, 12 outputs $\Rightarrow$ Hamiltonian matrix: 2976-by-2976



Example 1 (cont'd)

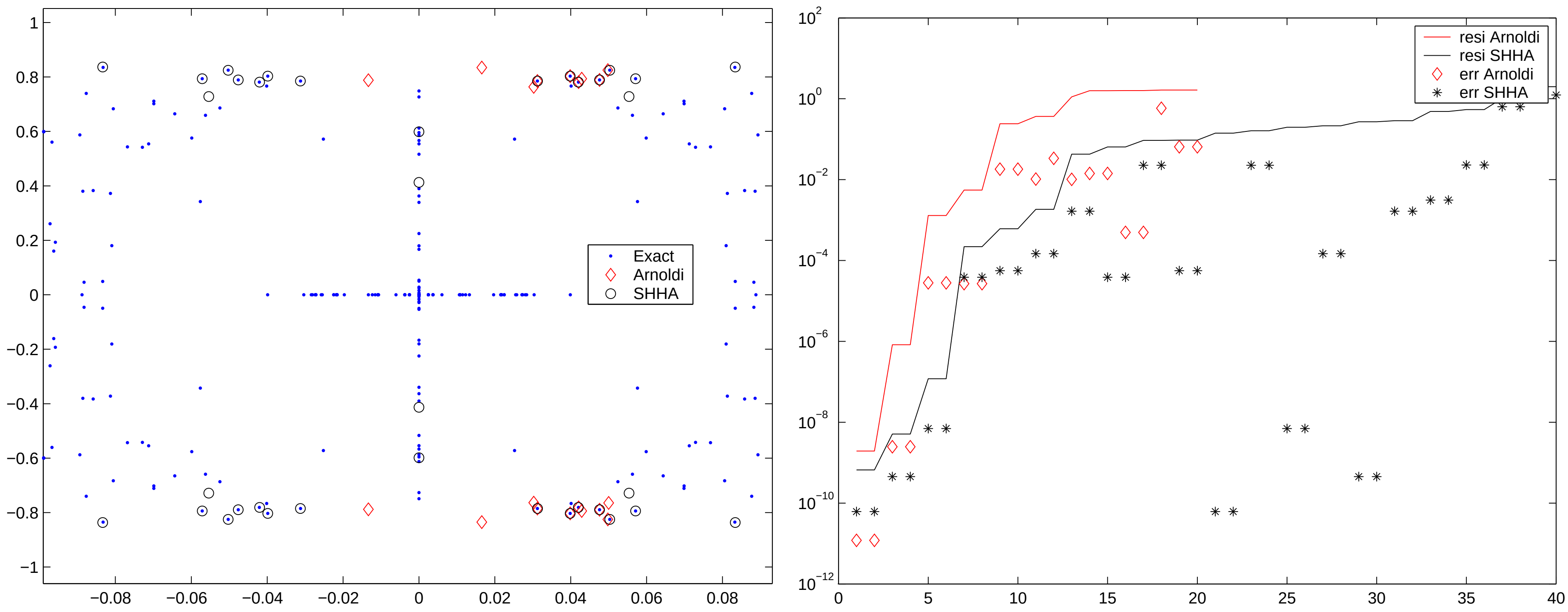
- $k = 20, \tau = 0.05 + 0.8j,$
- complex arithmetic: $A = (\mathcal{H} - \tau)^{-1}$





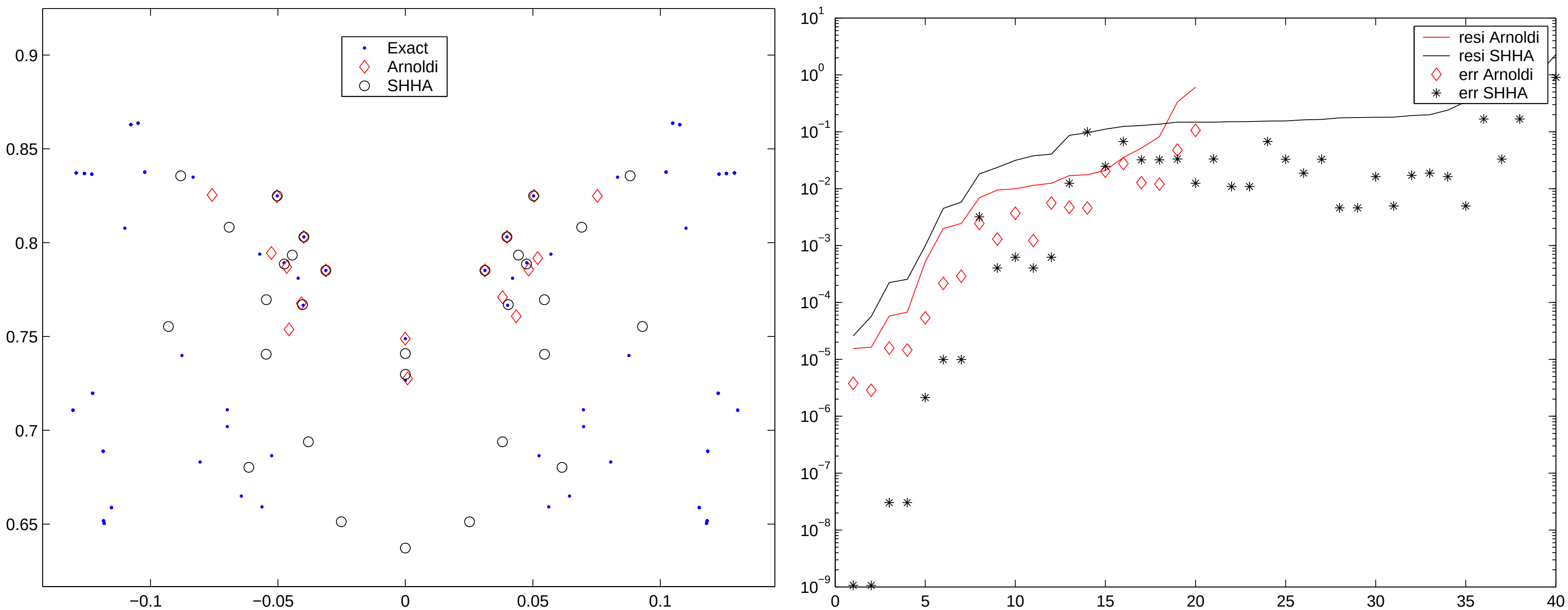
Example 1 (cont'd)

- $k = 20, \tau = 0.05 + 0.8j,$
- real arithmetic: $A = (\mathcal{H} - \tau)^{-1}(\mathcal{H} - \bar{\tau})^{-1}$



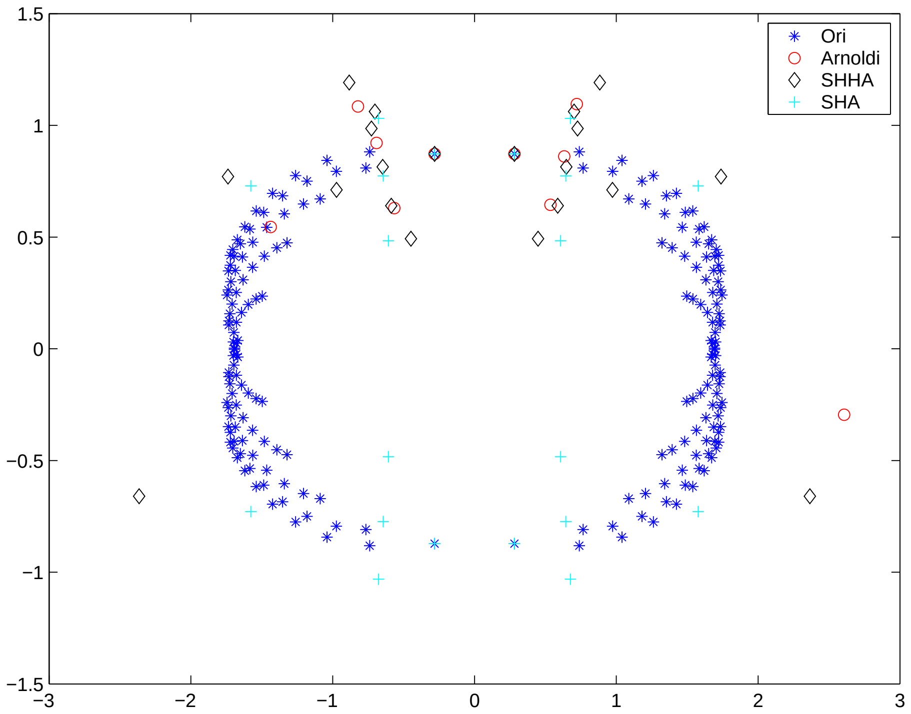
Example 1 (cont'd)

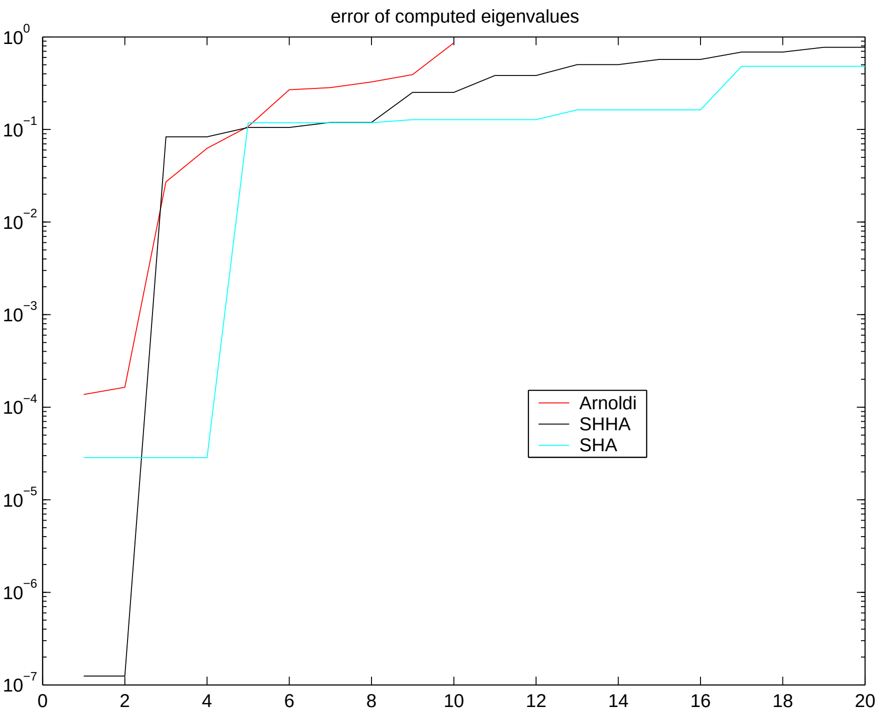
- $k = 20$, pure imaginary shift $\tau = 0.8j$,
- complex arithmetic: $A = (\mathcal{H} - \tau)^{-1}$



Example 2

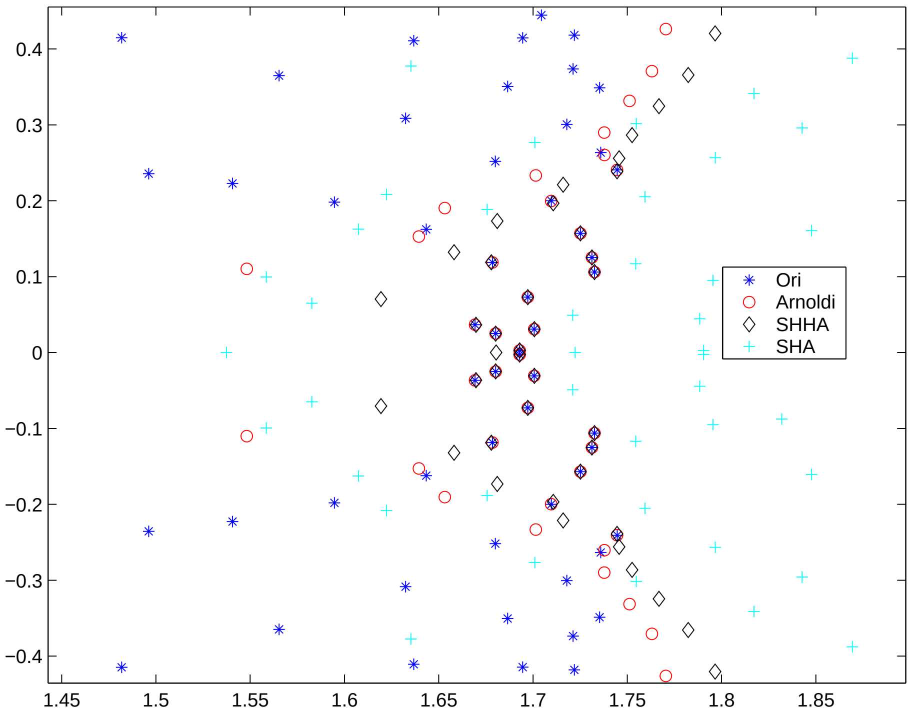
- Mehrmann and Watkins: SISC 2001, Example 6.1
- Pure imaginary $\tau = j$, $k = 10$ (as above)

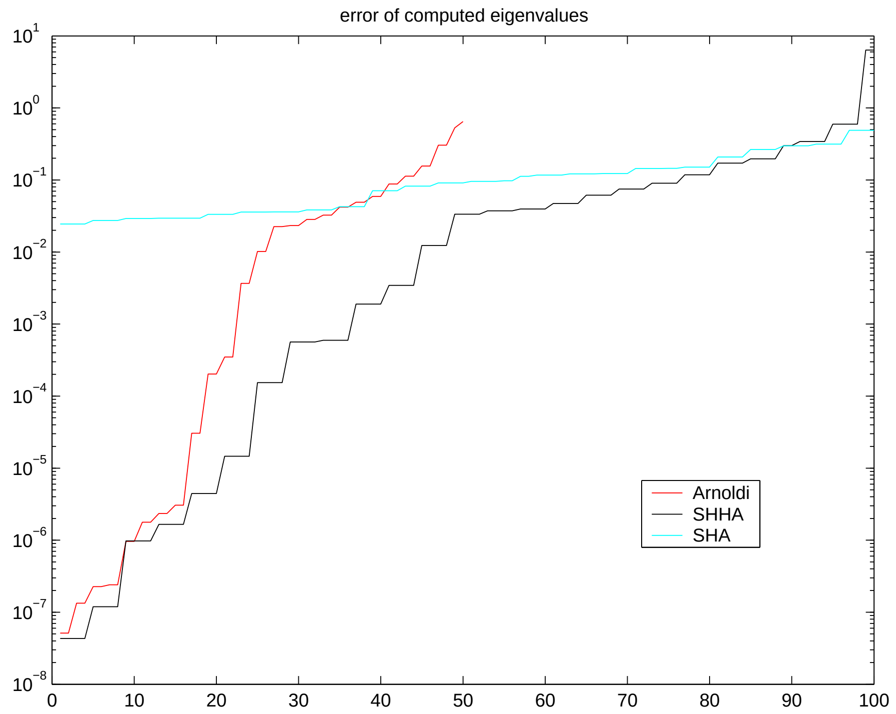




Example 2(cont'd)

- real $\tau = 1.85$, $k = 50$





Thanks!