Numerical algorithms for large-scale Hamiltonian eigenproblems

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Analysis, Algorithms, and Applications

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Definition

Let $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$, then $H \in \mathbb{R}^{2n\times 2n}$ is called Hamiltonian, if $(HJ)^T = HJ$.

Explicit block form of Hamiltonian matrices

$\begin{bmatrix} A & G \\ Q & -A^T \end{bmatrix}$, where $A, G, Q \in \mathbb{R}^{n\times n}$ and $G = G^T$, $Q = Q^T$.

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Hamiltonian Eigensymmetry

Hamiltonian matrices exhibit the Hamiltonian eigensymmetry:
if λ is a finite eigenvalue of H, then $\bar{\lambda}, -\lambda, -\bar{\lambda}$ are eigenvalues of H, too.

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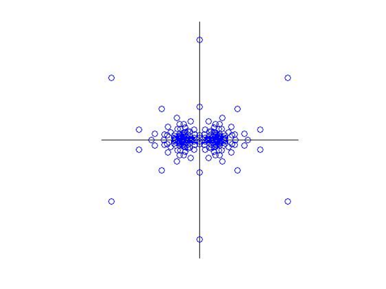
Typical Hamiltonian spectrum:



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Hamiltonian Eigenproblems

Goal

Structure-preserving algorithm, i.e., if $\tilde{\lambda}$ is a computed eigenvalue of H, then $\bar{\tilde{\lambda}}, -\tilde{\lambda}, -\bar{\tilde{\lambda}}$ should also be computed eigenvalues.

Goal cannot be achieved by general methods for matrices or matrix pencils like the QR, Lanczos, Arnoldi algorithms!

For an algorithm based on similarity transformations, the goal is achieved if the Hamiltonian structure is preserved.

Definition

$S \in \mathbb{R}^{2n \times 2n}$ is symplectic iff $\quad S^T J S = J, \quad$ i.e., $S^{-1} = J^T S^T J$.

Lemma

If H is Hamiltonian and S is symplectic, then

$$S^{-1} H S$$

is Hamiltonian, too.

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Hamiltonian eigenproblems arise in many different applications, e.g.:

- Systems and control
- Model reduction
- Computational physics:
  exponential integrators for Hamiltonian dynamics.
  [Eirola '03, Lopez/Simoncini '06]
- Quantum chemistry:
  computing excitation energies in many-particle systems using random phase approximation (RPA).
- Quadratic eigenvalue problems with Hamiltonian symmetry:
  - computation of corner singularities in 3D anisotropic elastic structures [Apel/Mehrmann/Watkins '01];
  - gyroscopic systems [Lancaster '99,...];
  - vibro-acoustics [Maess/Gaul '05];
  - optical waveguide design [Schmidt et al '03].

The Symplectic Lanczos Algorithm

Symplectic Lanczos Algorithm for Hamiltonian operators H

- is based on transpose-free unsymmetric Lanczos process [FREUND '94];
- computes partial J-tridiagonalization;
- provides a symplectic (J-orthogonal) Lanczos basis $V_k \in \mathbb{R}^{2n \times 2k}$, i.e., $V_k^T J_n V_k = J_k$;
- was derived in several variants: [FREUND/MEHRMANN '94, FERNG/LIN/WANG '97, B./FASSBENDER '97, WATKINS '04];
- requires re-J-orthogonalization using, e.g., modified symplectic Gram-Schmidt;
- can be restarted implicitly using implicit SR steps [B./FASSBENDER '97];
- exhibits convergence problems without locking & purging.

The Hamiltonian J-Tridiagonal Form

or Hamiltonian J-Hessenberg Form

$$T_n = \left[\begin{array}{ccccc|ccccc} \delta_1 & & & & & \beta_1 & \zeta_2 & & & \\ & \delta_2 & & & & \zeta_2 & \beta_2 & \zeta_3 & & \\ & & \delta_3 & & & & \zeta_3 & \ddots & \ddots & \\ & & & \ddots & & & & \ddots & \ddots & \zeta_n \\ & & & & \delta_n & & & & \zeta_n & \beta_n \\ \hline \nu_1 & & & & & -\delta_1 & & & & \\ & \nu_2 & & & & & -\delta_2 & & & \\ & & \nu_3 & & & & & -\delta_3 & & \\ & & & \ddots & & & & & \ddots & \\ & & & & \nu_n & & & & & -\delta_n \end{array}\right] \in \mathbb{R}^{2n\times 2n},$$

- can be computed by symplectic similarity $T_n = S^{-1}HS$ almost always,
- is computed partially by symplectic Lanczos process, based on symplectic Lanczos recursion

$$HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T, \qquad V_k = [S(:,1:k),\ S(:,n+1:n+k)].$$

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Theorem

If $T_n = S^{-1}HS$ is in Hamiltonian J-tridiagonal form, then

$$K(H, 2n-1, v) = SR \quad \text{with} \quad s_1 = v$$

is an SR decomposition of the Krylov matrix

$$K(H, 2n-1, v) := [v, Hv, \ldots, H^{2n-1}v].$$

If R is nonsingular, then T is unreduced, i.e., $\zeta_j \neq 0$ for all j.

Column-wise evaluation of $HS = ST_n$ yields ($S := [v_1, \ldots, v_n, w_1, \ldots, w_n]$)

$$\begin{aligned} Hv_k &= \delta_k v_k + \nu_k w_k \qquad \Longleftrightarrow \qquad \nu_k w_k = Hv_k - \delta_k v_k =: \widetilde{w}_k, \\ Hw_k &= \zeta_m v_{k-1} + \beta_k v_k - \delta_k w_k + \zeta_{k+1} v_{k+1} \\ &\Longleftrightarrow \qquad \zeta_{k+1} v_{k+1} = Hw_k - \zeta_k v_{k-1} - \beta_k v_k + \delta_k w_k =: \widetilde{v}_{k+1}. \end{aligned}$$

$\Longrightarrow$ Choose parameters $\delta_k, \beta_k, \nu_k, \zeta_k$ such that resulting algorithm computes symplectic (J-orthogonal) basis of Krylov subspace

$$\mathcal{K}(H, v_1, 2m) = \operatorname{span}\{v_1, Hv_1, \ldots, H^{2m-1}v_1\}.$$

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The Symplectic Lanczos Algorithm

Algorithm based on symplectic Lanczos recursion $HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T$

INPUT: $H \in \mathbb{R}^{2n \times 2n}$, $m \in \mathbb{N}$, and start vector $\tilde{v}_1 \neq 0 \in \mathbb{R}^{2n}$.

OUTPUT: $T_m \in \mathbb{R}^{2m \times 2m}$, $V_m \in \mathbb{R}^{2n \times 2m}$, ζ_{m+1}, and v_{m+1}.

1. $\zeta_1 = \|\tilde{v}_1\|_2$
2. $v_1 = \frac{1}{\zeta_1} \tilde{v}_1$
3. FOR $k = 1, 2, \ldots, m$
   - (a) $t = Hv_k$, $u = Hw_k$
   - (b) $\delta_k = \langle t, v_k \rangle$
   - (c) $\tilde{w}_k = t - \delta_k v_k$
   - (d) $\nu_k = \langle t, v_k \rangle_J$
   - (e) $w_k = \frac{1}{\nu_k} \tilde{w}_k$
   - (f) $\beta_k = -\langle u, w_k \rangle_J$
   - (g) $\tilde{v}_{k+1} = u - \zeta_k v_{k-1} - \beta_k v_k + \delta_k w_k$
   - (h) $\zeta_{k+1} = \|\tilde{v}_{k+1}\|_2$
   - (i) $v_{k+1} = \frac{1}{\zeta_{k+1}} \tilde{v}_{k+1}$

   ENDFOR

Note: 3(b) yields orthogonality of v_k, w_k [Ferng/Lin/Wang '97] and optimal conditioning of Lanczos basis [B. '03] if $\|v\|_2 = 1$ is forced.

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Extend Lanczos recursion by p symplectic Lanczos steps, yielding

$$HV_{k+p} = V_{k+p} T_{k+p} + \zeta_{k+p+1} v_{k+p+1} e_{2(k+p)}^T.$$

Let $S_{k+p} \in \mathbb{R}^{2(k+p)\times 2(k+p)}$ be symplectic. Then with

$$H \underbrace{(V_{k+p} S_{k+p})}_{\hat{V}_{k+p}} = \underbrace{(V_{k+p} S_{k+p})}_{\hat{V}_{k+p}} \underbrace{(S_{k+p}^{-1} T_{k+p} S_{k+p})}_{\hat{T}_{k+p}} + \zeta_{k+p+1} v_{k+p+1} e_{2(k+p)}^T S_{k+p},$$

$\hat{V}_{k+p}$ is J-orthogonal, $\hat{T}_{k+p}$ is Hamiltonian. Thus,

$$(*) \quad H\hat{V}_{k+p} = \hat{V}_{k+p} \hat{T}_{k+p} + \zeta_{k+p+1} v_{k+p+1} s_{k+p}^T \qquad (s_{k+p}^T := S_{k+p}(2(k+p), :)).$$

Obtain new Lanczos recursion from $(*)$ by truncating back to k and choosing S_{k+p} so that

- $\hat{T}_k$ is Hamiltonian J-tridiagonal,
- the residual term $\hat{\zeta}_{k+1} \hat{v}_{k+1} \hat{s}_k$ has the form vector $\times$ e_{2k}.

$\Longrightarrow$ implicit SR steps with structure-induced shift polynomials, e.g., $p_2(x) = (x-\mu)(x+\mu)$ or $p_4(x) = p_2(x)\overline{p_2(x)}$.

The Symplectic Lanczos Algorithm

Implicit Restarts for given k-step Lanczos recursion $HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T$.

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The SR Algorithm

Key Ingredients

- Bulge-chasing algorithm of GR class based on symplectic (J-orthogonal) similarity transformations. [Della-Dora '73]
- Algorithmic details analogous to QR algorithm, replace QR decomposition by SR (symplectic $\times$ "psychologically" upper triangular) decomposition, using orthosymplectic Givens and Householder as well as symplectic Gaussian eliminations. [Bunse-Gerstner/Mehrmann '86]
- Preserves the Hamiltonian J-tridiagonal form.
- Uses implicit double or quadruple shift SR steps which correspond to SR decomposition of $p_2(H) = (H - \mu I)(H + \mu I)$ or $p_4(H) = p_2(H)\overline{p_2(H)}$.
- Converges to Schur-like form with local cubic convergence rate. [Watkins/Elsner '91]
- Can be implemented using the $4n - 1$ parameters of the J-tridiagonal form only $\rightsquigarrow$ parametric SR algorithm. [Fassbender '07]

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SR iterates converge to

$$\left[\begin{array}{cccccc|cccccc}
A_1 & & & & & & G_1 & & & & & \\
& \ddots & & & & & & \ddots & & & & \\
& & A_k & & & & & & G_k & & & \\
& & & 0 & & & & & & G_{k+1} & & \\
& & & & \ddots & & & & & & \ddots & \\
& & & & & 0 & & & & & & G_m \\
\hline
0 & & & & & & -A_1^T & & & & & \\
& \ddots & & & & & & \ddots & & & & \\
& & 0 & & & & & & -A_k^T & & & \\
& & & Q_{k+1} & & & & & & 0 & & \\
& & & & \ddots & & & & & & \ddots & \\
& & & & & Q_m & & & & & & 0
\end{array}\right],$$

- the 1×1 blocks A_j represent real eigenvalues with $\lambda_j < 0$,
- the 2×2 blocks A_j represent complex eigenvalues with $\mathrm{Re}(\lambda_j) < 0$,
- the blocks $\begin{bmatrix} A_j & G_j \\ Q_j & -A_j^T \end{bmatrix}$ represent purely imaginary eigenvalues.
- Re-ordering of eigenvalues requires (block-)permutation only!

The SR Algorithm

Hamiltonian Schur-like form obtained from SR algorithm

SR iterates converge to

$$\left[\begin{array}{cccccc|cccccc}
A_1 & & & & & & G_1 & & & & & \\
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& & & 0 & & & & & & G_{k+1} & & \\
& & & & \ddots & & & & & & \ddots & \\
& & & & & 0 & & & & & & G_m \\
\hline
0 & & & & & & -A_1^T & & & & & \\
& \ddots & & & & & & \ddots & & & & \\
& & 0 & & & & & & -A_k^T & & & \\
& & & Q_{k+1} & & & & & & 0 & & \\
& & & & \ddots & & & & & & \ddots & \\
& & & & & Q_m & & & & & & 0
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- the 2×2 blocks A_j represent complex eigenvalues with $\mathrm{Re}(\lambda_j) < 0$,
- the blocks $\begin{bmatrix} A_j & G_j \\ Q_j & -A_j^T \end{bmatrix}$ represent purely imaginary eigenvalues.
- Re-ordering of eigenvalues requires (block-)permutation only!

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- To enhance convergence of implicitly restarted Krylov subspace methods need deflation strategies for
  - locking: deflate converged and wanted Ritz pairs,
  - purging: deflate converged but unwanted Ritz pairs,
- Deflation, locking & purging technically involved and hard to realize for implicitly restarted Arnoldi/Lanczos.
  [LEHOUCQ/SORENSEN '96, SORENSEN '02].
- Deflation strategies do not carry over to implicitly restarted symplectic Lanczos!
- Stewart's idea (SIMAX '01): rather than using Arnoldi decomposition (recursion), i.e.

  $$AV_k = V_k H_k + r_{k+1} e_k^T \quad \text{with upper Hessenberg matrix } H_k$$

  use Krylov-Schur decomposition

  $$AW_k = W_k T_k + r_{k+1} t_{k+1}^T \quad \text{with } T_k \text{ in (real) Schur form}$$

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Assume we have constructed a symplectic Lanczos decomposition of length $2(k+p) = 2m$ of the form

$$HV_m = V_m T_m + \zeta_{m+1} v_{m+1} e_{2m}^T.$$

Definition

$$H\hat{V}_m = \hat{V}_m \hat{T}_m + \hat{\zeta}_{m+1} \hat{v}_{m+1} \hat{s}_m^T$$

is a Hamiltonian Krylov-Schur-type decomposition if

- $\mathrm{rank}\left([\hat{V}_m, v_{m+1}]\right) = 2m+1,$
- $\hat{V}_m$ is J-orthogonal,
- $\hat{T}_m$ is in Hamiltonian Schur-type form.

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A Hamiltonian Krylov-Schur-Type Algorithm

Symplectic Lanczos decomposition ⇒ Hamiltonian Krylov-Schur-type decomposition

Applying *SR* algorithm to T_m yields symplectic matrix S_m such that $\hat{T}_m := S_m{}^{-1} T_m S_m$ has Hamiltonian Schur-like form.

As noted before, $\hat{T}_m$ can be ordered by *J*-orthogonal permutations so that converged and wanted/unwanted Ritz values appear in the leading/trailing blocks,

$$\hat{T}_m = \left[\begin{array}{cc|cc} A_1 & & G_1 & \\ & A_2 & & G_2 \\ \hline Q_1 & & -A_1^T & \\ & Q_2 & & -A_2^T \end{array}\right].$$

A Hamiltonian Krylov-Schur-Type Algorithm

Symplectic Lanczos decomposition ⇒ Hamiltonian Krylov-Schur-type decomposition

Applying SR algorithm to T_m yields symplectic matrix S_m such that $\hat{T}_m := {S_m}^{-1} T_m S_m$ has Hamiltonian Schur-like form ⇝

$$
\begin{aligned}
H(V_m S_m) &= (V_m S_m)(S_m^{-1} T_m S_m) + \zeta_{m+1} v_{m+1} e_{2m}^T S_m \\
&= [V_k, V_p, W_k, W_p] \left[\begin{array}{cc|cc} A_1 & & G_1 & \\ & A_2 & & G_2 \\ \hline Q_1 & & -A_1^T & \\ & Q_2 & & -A_2^T \end{array}\right] + \zeta_{m+1} v_{m+1} s_m^T
\end{aligned}
$$

Note: in case of deflation (⇝ locking possible), $s_m^T = [0, s_{p,1}^T, 0, s_{p,2}^T]$.

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\end{aligned}
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Purging: continue with Hamiltonian Krylov-Schur-type decomposition

$$
H[V_k, W_k] = [V_k, W_k] T_k + \zeta_{m+1} v_{m+1} s_k^T
$$

A Hamiltonian Krylov-Schur-Type Algorithm
Symplectic Lanczos decomposition ⇒ Hamiltonian Krylov-Schur-type decomposition

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Purging: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_k, W_k] = [V_k, W_k] T_k + \zeta_{m+1} v_{m+1} s_k^T$$

Locking: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_p, W_p] = [V_p, W_p] T_p + \zeta_{m+1} v_{m+1} s_p^T$$

A Hamiltonian Krylov-Schur-Type Algorithm

Symplectic Lanczos decomposition ⇒ Hamiltonian Krylov-Schur-type decomposition

Applying SR algorithm to T_m yields symplectic matrix S_m such that $\hat{T}_m := {S_m}^{-1} T_m S_m$ has Hamiltonian Schur-like form

$$\begin{aligned} H(V_m S_m) &= (V_m S_m)(S_m^{-1} T_m S_m) + \zeta_{m+1} v_{m+1} e_{2m}^T S_m \\ &= [V_k, V_p, W_k, W_p] \left[\begin{array}{cc|cc} A_1 & & G_1 & \\ & A_2 & & G_2 \\ \hline Q_1 & & -A_1^T & \\ & Q_2 & & -A_2^T \end{array}\right] + \zeta_{m+1} v_{m+1} s_m^T \end{aligned}$$

Note: in case of deflation ($\rightsquigarrow$ locking possible), $s_m^T = [0, s_{p,1}^T, 0, s_{p,2}^T]$.

Purging: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_k, W_k] = [V_k, W_k] T_k + \zeta_{m+1} v_{m+1} s_k^T$$

Locking: continue with Hamiltonian Krylov-Schur-type decomposition

$$H[V_p, W_p] = [V_p, W_p] T_p + \zeta_{m+1} v_{m+1} s_p^T$$

In order to expand subspace back to length m, need to return to symplectic Lanczos decomposition!

A Hamiltonian Krylov-Schur-Type Algorithm

Hamiltonian Krylov-Schur-type decomposition $\Rightarrow$ symplectic Lanczos decomposition

Theorem

Every Hamiltonian Krylov-Schur-type decomposition is equivalent to a symplectic Lanczos decomposition.

Constructive proof:

Given a Hamiltonian Krylov-Schur-type decomposition of length k,

$$HU = UT + us^T.$$

1. J-orthogonalize u w.r.t. U so that $U^T Ju = 0 \;\Rightarrow \hat{u} := \frac{1}{\gamma}(u - Ut)$,

$$HU = UT + (\gamma\hat{u} + Ut)s^T = U(T + ts^T) + \gamma\hat{u}s^T =: UB + \hat{u}\hat{s}^T.$$

Theorem

Every Hamiltonian Krylov-Schur-type decomposition is equivalent to a symplectic Lanczos decomposition.

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Given a Hamiltonian Krylov-Schur-type decomposition of length k,

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1. J-orthogonalize u w.r.t. U so that $U^T Ju = 0 \;\Rightarrow\; HU = UB + \hat{u}\hat{s}^T$.
2. Compute orthogonal symplectic matrix W such that $W^T\hat{s} = \hat{\zeta}e_{2k}^T \Rightarrow$

$$HUW = UW(W^TBW) + \hat{u}\hat{s}^TW =: UW\tilde{B} + \hat{\zeta}\hat{u}e_{2k}^T.$$

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$$HUW = UW\tilde{B} + \hat{\zeta}\hat{u}e_{2k}^T.$$
3. Compute symplectic matrix S restoring J-tridiagonal form of $\tilde{B}$, i.e., $S^{-1}\tilde{B}S = \hat{T}$ is Hamiltonian J-tridiagonal and $e_{2k}^T S = e_{2k}^T$ (⇝ row-wise bottom-to-top J-tridiagonalization) ⇒
$$H\underbrace{UWS}_{=:V} = \underbrace{UWS}_{=:V}\underbrace{S^{-1}\tilde{B}S}_{=\hat{T}} + \hat{\zeta}\hat{u}e_{2k}^T$$
is an equivalent symplectic Lanczos decomposition.

Algorithm HKS

1. Use k steps of symplectic Lanczos process to compute symplectic Lanczos decomposition

$$HV_k = V_k T_k + \zeta_{k+1} v_{k+1} e_{2k}^T.$$

2. Expand Krylov subspace to length $2(k+p)$ using p steps of symplectic Lanczos process,

$$HV_{k+p} = V_{k+p} T_{k+p} + \zeta_{k+p+1} v_{k+p+1} e_{2(k+p)}^T.$$

3. Run (parametrized) SR algorithm on T_{k+p} to obtain Hamiltonian Krylov-Schur type decomposition

$$HU_{k+p} = U_{k+p} \tilde{T}_{k+p} + \zeta_{k+p+1} v_{k+p+1} s_{k+p}^T.$$

4. Re-order Hamiltonian Schur-type form as desired, deflate/purge, yielding new Hamiltonian Krylov-Schur type decomposition

$$H\tilde{U}_k = \tilde{U}_k \tilde{T}_k + \tilde{\zeta}_{k+1} \tilde{v}_{k+1} \tilde{s}_k^T.$$

(In case of deflation of ℓ converged Ritz values, $k \leftarrow k - \ell$.)

5. Compute equivalent symplectic Lanczos decomposition

$$H\hat{V}_k = \hat{V}_k \hat{T}_k + \hat{\zeta}_{k+1} \hat{v}_{k+1} e_{2k}^T.$$

6. IF $k > 0$, GOTO 2.

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Quadratic Eigenproblems with Hamiltonian Symmetry

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

$$\text{where } M = M^T,\ K = K^T,\ G = -G^T,$$

can be solved using linearization

$$\left(\lambda \begin{bmatrix} M & 0 \\ 0 & I \end{bmatrix} - \begin{bmatrix} -G & -K \\ I & 0 \end{bmatrix}\right) \begin{bmatrix} y \\ x \end{bmatrix} = 0 \qquad (y := \lambda x).$$

$\rightsquigarrow$ unstructured (generalized) eigenproblem, spectral symmetry is destroyed in finite precision computations.

Quadratic Eigenproblems with Hamiltonian Symmetry

$$Q(\lambda)x := (\lambda^2 M + \lambda G + K)x = 0,$$
$$\text{where } M = M^T,\ K = K^T,\ G = -G^T,$$

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$$(\lambda N - H)\,z = \left(\lambda \begin{bmatrix} I & G \\ 0 & I \end{bmatrix} - \begin{bmatrix} 0 & -K \\ M^{-1} & 0 \end{bmatrix}\right) \begin{bmatrix} y \\ x \end{bmatrix} = 0 \quad (y := \lambda M x)$$

$\rightsquigarrow$ skew-Hamiltonian/Hamiltonian eigenproblem, i.e., N is skew-Hamiltonian ($(NJ)^T = -(NJ)^T$), H is Hamiltonian;

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$\rightsquigarrow$ skew-Hamiltonian/Hamiltonian eigenproblem, i.e., N is skew-Hamiltonian ($(NJ)^T = -(NJ)^T$), H is Hamiltonian;

$\rightsquigarrow$ spectral symmetry can be preserved in finite precision computations if structure-preserving algorithm is used!

$\rightsquigarrow$ Skew-Hamiltonian Implicitly Restarted Arnoldi (SHIRA) [Mehrmann/Watkins '01].

Quadratic Eigenproblems with Hamiltonian Symmetry

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$\rightsquigarrow$ skew-Hamiltonian/Hamiltonian eigenproblem, i.e., N is skew-Hamiltonian ($(NJ)^T = -(NJ)^T$), H is Hamiltonian;

Skew-Hamiltonian/Hamiltonian eigenproblem is equivalent to Hamiltonian eigenproblem $Hz = \lambda z$ with

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

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For eigenvalues of largest magnitude apply HKS to

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

For eigenvalues of smallest magnitude apply HKS to

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

Note: more efficient than SHIRA applied to H^{-2}!

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For eigenvalues of smallest magnitude apply HKS to

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

For interior real/purely imaginary eigenvalues apply HKS to

$$\begin{aligned} H_2(\tau) &= HR_2(\tau) = H(H-\tau I)^{-1}(H+\tau I)^{-1} \\ &= \begin{bmatrix} -\frac{1}{2}G & -K \\ I & 0 \end{bmatrix} \begin{bmatrix} I & \tau I \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & I \\ -Q(\tau)^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & G \\ 0 & I \end{bmatrix} \\ &\quad \times \begin{bmatrix} 0 & I \\ -Q(\tau)^{-T} & 0 \end{bmatrix} \begin{bmatrix} I & -\tau I \\ 0 & I \end{bmatrix} \begin{bmatrix} I & \frac{1}{2}G \\ 0 & M \end{bmatrix}. \end{aligned}$$

Applying $Q(\tau)^{-1}, Q(\tau)^{-T}$ requires only 1 LU factorization!

Note: as efficient as SHIRA applied to $R_2(\tau)$!

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For eigenvalues of largest magnitude apply HKS to

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For interior complex eigenvalues apply HKS to

$$\begin{aligned} H_4(\tau) &= HR_4(\tau) \\ &= H(H-\tau I)^{-1}(H+\tau I)^{-1}(H-\overline{\tau} I)^{-1}(H+\overline{\tau} I)^{-1}. \end{aligned}$$

Note: as efficient as SHIRA applied to $R_4(\tau)$!

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- We apply `eigs` and HKS (and SHIRA for nonzero shifts) to several test sets.
- Convergence is based on comparable stopping criteria: Ritz values are taken as converged if relative residuals for the shift-and-invert operators are smaller than given tolerance.
- Relative residuals in numerical examples are the residuals for the QEP, i.e.,

$$\frac{\|(\tilde{\lambda}^2 M + \tilde{\lambda} G + K)\tilde{x}\|_1}{\|\tilde{\lambda}^2 M + \tilde{\lambda} G + K\|_1 \|\tilde{x}\|_1},$$

where $(\tilde{\lambda}, \tilde{x})$ is a converged Ritz pair.

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- Here: 3D elasticity problem for Fichera corner (cutting the cube $[0,1] \times [0,1] \times [0,1]$ out of the cube $(-1,1) \times (-1,1) \times (-1,1)$).
- $n = 12,828$, matrix assembly with software *CoCoS* [C. Pester '05].
- Want 12 eigenvalues closest to target shift $\tau = 1$.
- Compare SHIRA applied to $R_2(1)$, `eigs` and HKS applied to $H_2(1)$.
- SHIRA needs 3, `eigs` 6, HKS 4 iterations.
- Max. condition number in SR iterations: $\max(\mathrm{cond}\,(SR)) = 3.35 \cdot 10^5$.

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SHIRA		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
0.90510929898162	$2 \cdot 10^{-14}$	0.90510929894951	$6 \cdot 10^{-16}$
0.90529568786502	$2 \cdot 10^{-14}$	0.90529568784944	$5 \cdot 10^{-16}$
1.07480595544983	$5 \cdot 10^{-15}$	1.07480595544985	$4 \cdot 10^{-16}$
1.60117345104537	$1 \cdot 10^{-13}$	1.60117345101134	$6 \cdot 10^{-16}$
1.65765608689959	$4 \cdot 10^{-14}$	1.65765608679830	$3 \cdot 10^{-15}$
1.65914529725492	$1 \cdot 10^{-14}$	1.65914529702482	$7 \cdot 10^{-15}$

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`eigs`		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
0.90510929898127	$4\cdot 10^{-16}$	0.90510929894951	$6\cdot 10^{-16}$
0.90529568786417	$4\cdot 10^{-16}$	0.90529568784944	$5\cdot 10^{-16}$
1.07480595545002	$4\cdot 10^{-16}$	1.07480595544985	$4\cdot 10^{-16}$
1.60117345102312	$2\cdot 10^{-16}$	1.60117345101134	$6\cdot 10^{-16}$
1.65765608688689	$2\cdot 10^{-16}$	1.65765608679830	$3\cdot 10^{-15}$
1.65914529726339	$1\cdot 10^{-16}$	1.65914529702482	$7\cdot 10^{-15}$

Numerical Examples

Gyroscopic systems: rolling tire

- Modeling the noise of rolling tires requires to determine the transient vibrations, [Nackenhorst/von Estorff '01].
- FEM model of a deformable wheel rolling on a rigid plane surface results in a gyroscopic system of order $n = 124,992$ [Nackenhorst '04].
- Sparse LU factorization of $Q(\tau)$ requires about 6 GByte.
- Here, use reduced-order model of size $n = 2,635$ computed by AMLS [Elssel/Voss '06].

Numerical Examples

Gyroscopic systems: rolling tire

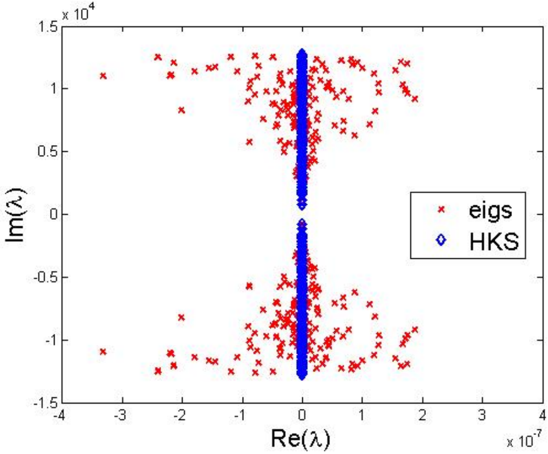
- Compare `eigs` and HKS applied to H^{-1} to compute the 12 smallest eigenvalues.
- `eigs` needs 8, HKS 6 iterations.
- $\max(\mathrm{cond}\,(SR)) = 331$.
- Eigenvalues scaled by 1,000.

`eigs`		HKS	
Eigenvalue	Residual	Eigenvalue	Residual
$4 \cdot 10^{-12} + 1.73705142673\imath$	$2 \cdot 10^{-14}$	$1.73705142671\imath$	$5 \cdot 10^{-17}$
$-3 \cdot 10^{-12} + 1.66795405953\imath$	$8 \cdot 10^{-15}$	$1.66795405955\imath$	$2 \cdot 10^{-15}$
$2 \cdot 10^{-13} + 1.66552788164\imath$	$2 \cdot 10^{-15}$	$1.66552788164\imath$	$1 \cdot 10^{-16}$
$4 \cdot 10^{-14} + 1.58209209804\imath$	$1 \cdot 10^{-16}$	$1.58209209804\imath$	$5 \cdot 10^{-17}$
$-1 \cdot 10^{-14} + 1.13657108578\imath$	$8 \cdot 10^{-17}$	$1.13657108578\imath$	$7 \cdot 10^{-18}$
$1 \cdot 10^{-14} + 0.80560062107\imath$	$1 \cdot 10^{-16}$	$0.80560062107\imath$	$6 \cdot 10^{-18}$

Numerical Examples

Gyroscopic systems: rolling tire

- Compare `eigs` and HKS applied to H^{-1} to compute the 180 smallest eigenvalues.



Conclusions and Outlook

Conclusions

- Solution of large-scale eigenproblems with Hamiltonian eigensymmetry in a numerically reliable way possible by combination of symplectic Lanczos process and Krylov-Schur restarting.
- Alternative to SHIRA, often with faster convergence.
- Relies on parameterized SR algorithm [FASSBENDER '07].
- Advantageous in particular in presence of eigenvalues on the imaginary axis, e.g., for stable gyroscopic systems.

Conclusions and Outlook

Outlook

- Integration into HAPACK ($\equiv$ better and more reliable implementation. . .)
- Comparison to SOAR [Bai/Su '05] for second-order eigenproblems.
- Solution of higher-order, structured polynomial eigenproblems.
- Rational Krylov methods for Hamiltonian eigenproblems; RatSHIRA developed by C. Effenberger (diploma thesis, TU Chemnitz 2008).
- Version for symplectic/palindromic eigenproblems based on symplectic Lanczos process and SZ iteration.
- Two-sided symplectic (implicitly restarted) Arnoldi based on symplectic URV decomposition [B./Kressner/Mehrmann/Xu], soon.

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