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THE SYMPLECTIC LANCZOS PROCESS FOR HAMILTONIAN-POSITIVE MATRICES

(Symplectic Lanczos for Hamiltonian-positive matrices encounters no serious breakdown!)

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Introduction

Hamiltonian Eigenproblems

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 $(HJ)^T = HJ$.

Note: $J^{-1} = J^T = -J$.

Explicit block form of Hamiltonian matrices

$$\begin{bmatrix} A & B \\ C & -A^T \end{bmatrix}, \quad \text{where } A, B, C \in \mathbb{R}^{n \times n} \quad \text{and } B = B^T,\ C = C^T.$$

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Spectral Properties

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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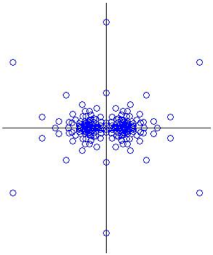
Typical Hamiltonian spectrum



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/QZ, Lanczos, Arnoldi algorithms!

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

Definition

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

$V_k \in \mathbb{R}^{2n \times 2k}$ is symplectic or a J-isometry if $\quad V_k^T J_n V_k = J_k$.

Lemma

If H is Hamiltonian and V is symplectic, then $V^{-1} H V$ is Hamiltonian, too.

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If H is Hamiltonian and V is symplectic, then $V^{-1}HV$ is Hamiltonian, too.

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Applications

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

- Systems and control:
  - Solution methods for algebraic and differential Riccati equations.
  - Design of LQR/LQG/H_2/H_∞ controllers and filters for continuous-time linear control systems.
  - Stability radii and system norm computations; optimization of system norms.
  - Passivity-preserving model reduction based on balancing.
  - Reduced-order control for infinite-dimensional systems based on inertial manifolds.
- Computational physics:
  exponential integrators for Hamiltonian dynamics.
  [Eirola '03, Lopez/Simoncini '06, B./Meister '13]
- Quantum chemistry:
  computing excitation energies in many-particle systems using random phase approximation (RPA).
- Quadratic eigenvalue problems:
  in particular, gyroscopic systems.

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] or Krylov-Schur restarting [B./FASSBENDER/STOLL '11] which allows easy locking & purging procedure;
- does not provide an orthogonal Lanczos basis and is prone to serious breakdown.

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 $T_n = V^{-1}HV$ for almost (serious breakdown!) any $V_1 = V(:,1)$,
- is computed partially by symplectic Lanczos process, based on symplectic Lanczos recursion

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

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: $H \in \mathbb{R}^{2n\times 2n}$, $k \in \mathbb{N}$, and start vector $\tilde{v}_1 \neq 0 \in \mathbb{R}^{2n}$.
OUTPUT: $T_k \in \mathbb{R}^{2k\times 2k}$, $V_k \in \mathbb{R}^{2n\times 2k}$, ζ_{k+1}, and v_{k+1}.

1. $\zeta_1 = \|\tilde{v}_1\|_2$
2. $v_1 = \frac{1}{\zeta_1}\tilde{v}_1$
3. FOR $m = 1, 2, \ldots, k$
   (a) $t = Hv_m$
   (b) $\delta_m = \langle t, v_m\rangle$ `% B./Faßbender '97:` $\delta_m = 1$, `Watkins '04:` $\delta_m = 0$.
   (c) $\tilde{w}_m = t - \delta_m v_m$
   (d) $\nu_m = \langle t, v_m\rangle_J$
   (e) $w_m = \frac{1}{\nu_m}\tilde{w}_m$
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   (h) $\tilde{v}_{m+1} = u - \zeta_m v_{m-1} - \beta_m v_m + \delta_m w_m$
   (i) $\zeta_{m+1} = \|\tilde{v}_{m+1}\|_2$
   (j) $v_{m+1} = \frac{1}{\zeta_{m+1}}\tilde{v}_{m+1}$

   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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The Symplectic Lanczos Algorithm

Numerical example: rolling tire **Results from** [B./Fassbender/Stoll '08/'11]

- 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].
- Here, use reduced-order model of size $n = 2,635$ computed by AMLS [Elssel/Voss '06].

The Symplectic Lanczos Algorithm

Numerical example: rolling tire **Results from** [B./Fassbender/Stoll '08/'11]

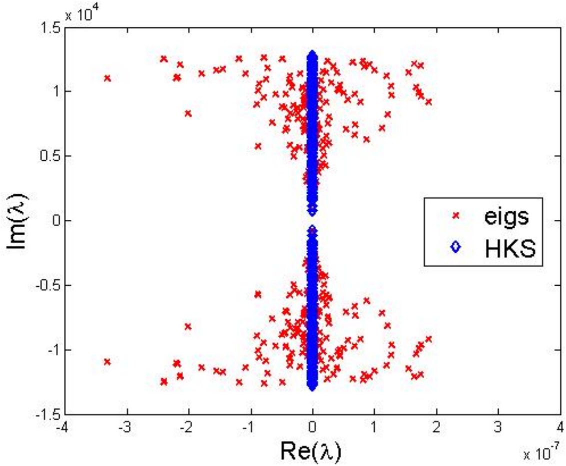
- Compare eigs and symplectic Lanczos with Krylov-Schur restarting (HKS) applied to H^{-1} to compute the 12 smallest eigenvalues.
- eigs needs 8, HKS 6 iterations.
- $\max(\mathrm{cond}\,(SR)) = 331$.
- Eigenvalues scaled by 1,000.

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

The Symplectic Lanczos Algorithm

Numerical example: rolling tire **Results from** [B./FASSBENDER/STOLL '08/'11]

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



Symplectic Lanczos for Hamiltonian-positive Matrices

Hamiltonian-positive Matrices

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A Hamiltonian matrix $H \in \mathbb{R}^{2n \times 2n}$ is called Hamiltonian-positive if its symmetric generator $S = J^T H$ is positive definite.

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Lemma [Amodio 2003]

All eigenvalues of Hamiltonian-positive matrices are purely imaginary, i.e., $\Lambda(H) \subset \jmath\mathbb{R}$.

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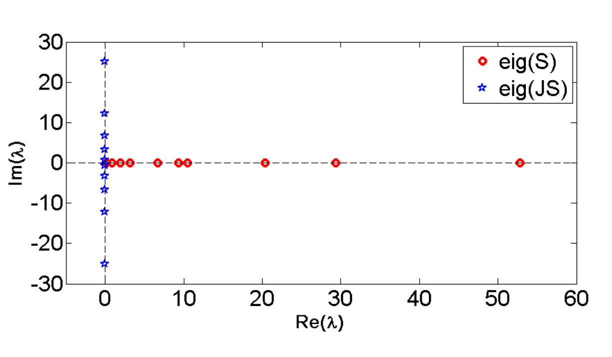
Comparison of spectra of spd generator and its Hamiltonian



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Example: weakly coupled Hamiltonian systems

$$\begin{array}{rcl} \dot{p} & = & \mathcal{H}_q, \\ \dot{q} & = & -\mathcal{H}_p, \end{array} \qquad \text{for Hamiltonian } \mathcal{H}(p,q) = \frac{1}{2}\left(p^T p + q^T K q + 2p^T W q\right)$$

with kinetic energy determined by $K = K^T > 0$ and weak coupling, i.e., $\|W\|$ "small" $\rightsquigarrow$

$$S = J^T H = \begin{bmatrix} I_n & W \\ W^T & K \end{bmatrix} > 0 \quad \text{if } \|W\| \text{ "small" enough.}$$

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Remark: Hamiltonian-positiveness of T_k can be enforced; $\beta_m = -\langle u, w_m \rangle_J = -u^T S u < 0$.

How About Symplectic Arnoldi?

Hamiltonian-positive Matrices

Symplectic Arnoldi recursion

$$HV_k = V_k H_k + \zeta_k v_{k+1},$$

where V_k is symplectic and orthogonal, H_k is in Hamiltonian Hessenberg form:

$$H_k = \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & -H_{11}^T \end{bmatrix} \text{ with } H_{11} = \left[\quad\right], \; H_{12} = H_{12}^T, \; H_{21} = h_{k+1,k} e_k e_k^T.$$

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Theorem [AMMAR/MEHRMANN '91]

There exists a symplectic Arnoldi reduction with H_n unreduced, i.e., $h_{j+1,j} \neq 0$, if and only if $\exists$ x with

$$x^T J H^{2k-1} x = 0 \; (k = 1, 2, \ldots, n-1), \quad x^T x = 1,$$

that is not contained in an H-invariant subspace of dimension $\leq n$.

For H Hamiltonian-positive, no such vector exists!
(Already observed in [AMMAR/MEHRMANN '91, page 65].)

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