Structured Krylov Subspace Methods for Eigenproblems with Spectral Symmetries

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Overview

- The Hamiltonian eigenproblem
- Applications
- The symplectic Lanczos method
- Choosing the free parameters
- Numerical examples
- Conclusions

The Hamiltonian Eigenproblem

$$Hx = \lambda x$$

$H \in \mathbb{R}^{2n\times 2n}$ is a Hamiltonian matrix, i.e., $(HJ)^T = HJ$, where $J = \left[\begin{smallmatrix} 0 & I_n \\ -I_n & 0 \end{smallmatrix}\right]$.

Hamiltonian matrices

- have explicit block structure implied by symmetry of HJ,

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

- are skew-selfadjoint w.r.t. indefinite inner product $\langle x, y\rangle_J := x^T J y$.
- form Lie algebra with corresponding Lie group:

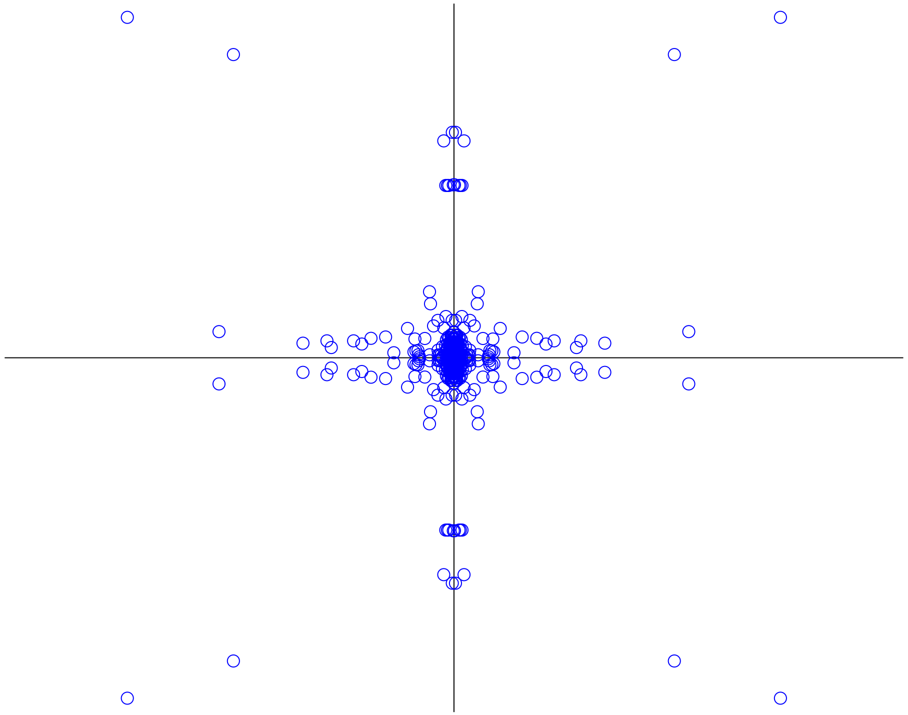
$$\mathcal{S}_n := \{S \in \mathbb{R}^{2n\times 2n} \mid SJS^T = J\} = \text{ symplectic matrices},$$

hence $S^{-1}HS$ is Hamiltonian for all $S \in \mathcal{S}_{2n}$.

Spectral Properties

Spectral symmetry with respect to real and imaginary axes:

$$\lambda \in \Lambda(H) \;\Rightarrow\; -\lambda, \pm\overline{\lambda} \in \Lambda(H)$$



Hence,

- $\lambda \in \mathbb{R} \Rightarrow \pm\lambda \in \Lambda(H)$,
- $\lambda = \jmath\omega \in \jmath\mathbb{R} \Rightarrow \pm\jmath\omega \in \Lambda(H)$,
- $\lambda \in \mathbb{C} \setminus \jmath\mathbb{R} \Rightarrow \pm\lambda, \pm\overline{\lambda} \in \Lambda(H)$,

Applications

- 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-dim. systems based on inertial manifolds.
- Computational physics: exponential inegrators for Hamiltonian dynamics.
- Quantum chemistry: computing excitation energies in many-particle systems using random phase approximation (RPA).
- Quadratic eigenvalue problems...

Quadratic Eigenvalue Problems

Consider

$$\lambda^2 Mx + \lambda Gx + Kx = 0,$$

where $M = M^T$ spd, $K = K^T$, $G = -G^T$.

Motivation:

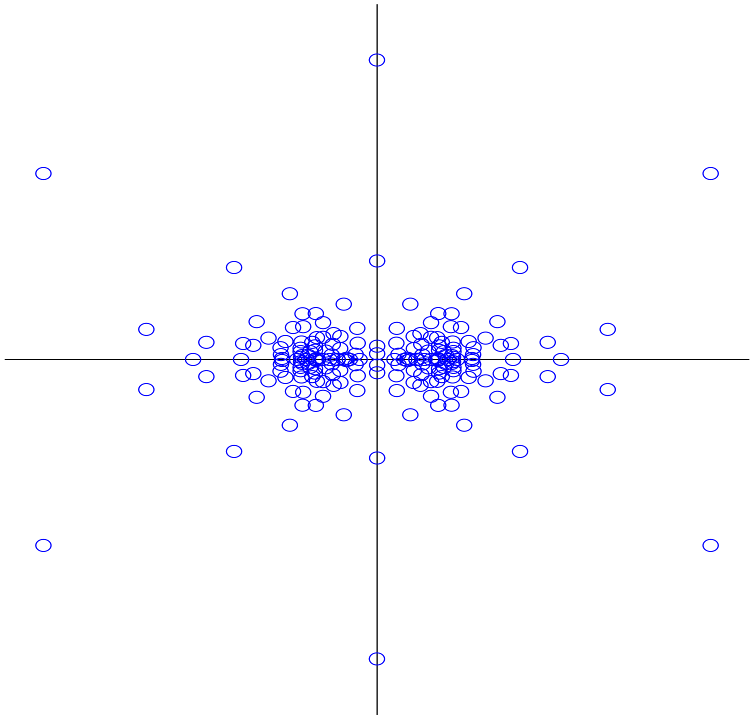
- linear elasticity: computation of corner singularities in 3D anisotropic elastic structures [Apel/Mehrmann/Watkins '01]
- FE discretization in structural analysis [H.R. Schwarz '84]
- acoustic simulation of poro-elastic materials [Meerbergen '99]
- gyroscopic systems, rotor systems [Lancaster '99]

Spectral Symmetry of QEP

Spectrum of matrix polynomial

$$\lambda^2 Mx + \lambda Gx + Kx = 0, \qquad G = -G^T,$$

looks like



$\Rightarrow$ Hamiltonian symmetry!

Linearization of QEP

Setting $y = \lambda x$ yields linear (generalized) eigenvalue problem

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

$H = \begin{bmatrix} 0 & -K \\ M & 0 \end{bmatrix}$ is Hamiltonian: $(HJ)^T = HJ$

$N = \begin{bmatrix} M & G \\ 0 & M \end{bmatrix}$ is skew-Hamiltonian: $(NJ)^T = -NJ$

$\Longrightarrow H - \lambda N$ is a Hamiltonian/skew-Hamiltonian pencil [Mehrmann/Watkins '00]

Re-formulation of $H - \lambda N$

Note:

$$N = Z_1 Z_2 = \left[\begin{array}{cc} I & \frac{1}{2}G \\ 0 & M \end{array}\right] \left[\begin{array}{cc} M & \frac{1}{2}G \\ 0 & I \end{array}\right].$$

Hence, as M is spd

$$Z_1^{-1}(H - \lambda N) Z_2^{-1} = W - \lambda I,$$

where

$$W = \left[\begin{array}{cc} I & -\frac{1}{2}G \\ 0 & I \end{array}\right] \left[\begin{array}{cc} 0 & -K \\ M^{-1} & 0 \end{array}\right] \left[\begin{array}{cc} I & -\frac{1}{2}G \\ 0 & I \end{array}\right]$$

W is Hamiltonian!

Structured Lanczos Method for Hamiltonian Matrices

Observations:

- Preservation of spectral symmetry requires structured eigensolver.
- Hamiltonian structure is preserved under symplectic similarity transformations.
- For large, sparse problems want Krylov subspace method.

$\Longrightarrow$ Need symplectic basis for Krylov subspace

$$\mathcal{K}(H, 2k, v) := \mathrm{span}\{v, Hv, H^2 v, \ldots, H^{2k-1}\}.$$

H nonsymmetric $\rightsquigarrow$ apply Arnoldi method or nonsymmetric Lanczos method.

Arnoldi method can only produce symplectic Krylov basis in very particular instances! [Ammar/Mehrmann '91] $\Longrightarrow$ Need variant of nonsymmetric Lanczos!

Symplectic Lanczos Transformation

For every Hamiltonian matrix H there exists symplectic similarity transformation

$$\widetilde{H} = S^{-1}HS = \left[\begin{array}{ccccc|ccccc}
\delta_1 & & & & & \beta_1 & \zeta_2 & & & \\
& \delta_2 & & & & \zeta_2 & \beta_2 & \zeta_3 & & \\
& & \delta_3 & & & & \zeta_3 & \ddots & \ddots & \\
& & & \ddots & & & & \ddots & \ddots & \zeta_n \\
& & & & \delta_n & & & & \zeta_n & \beta_n \\
\hline
\nu_1 & & & & & -\delta_1 & & & & \\
& \nu_2 & & & & & -\delta_2 & & & \\
& & \nu_3 & & & & & -\delta_3 & & \\
& & & \ddots & & & & & \ddots & \\
& & & & \nu_n & & & & & -\delta_n
\end{array}\right]$$

Hamiltonian J-tridiagonal (J-Hessenberg) form

$\Longrightarrow$ Need $4n-1$ parameters to represent $\widetilde{H}$.

Relation of Reduced Form and Krylov Subspace

Theorem:

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

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

is an SR decomposition of the Krylov matrix

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

Some Notation

Permutation using $P := [e_1, e_3, \ldots, e_{2n-1}, e_2, e_4, \ldots, e_{2n}]$ (perfect shuffle) yields

$$H_P \quad := \quad PHP^T, \quad S_P := PSP^T, \quad J_P := PJP^T = \mathrm{diag}\left(\left[\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right], \ldots, \left[\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right]\right)$$

$$\widetilde{H}_P \quad := \quad S_P^{-1} H_P S_P = \left[\begin{array}{cc|cc|cc|cc|cc}
\delta_1 & \beta_1 & 0 & \zeta_2 & & & & & & \\
\nu_1 & -\delta_1 & 0 & 0 & & & & & & \\ \hline
0 & \zeta_2 & \delta_2 & \beta_2 & 0 & \zeta_3 & & & & \\
0 & 0 & \nu_2 & -\delta_2 & 0 & 0 & & & & \\ \hline
 & & 0 & \zeta_3 & \ddots & & \ddots & & & \\
 & & 0 & 0 & & \ddots & & \ddots & & \\ \hline
 & & & & \ddots & & \ddots & & 0 & \zeta_n \\
 & & & & & \ddots & & \ddots & 0 & 0 \\ \hline
 & & & & & & 0 & \zeta_n & \delta_n & \beta_n \\
 & & & & & & 0 & 0 & \nu_n & -\delta_n
\end{array}\right]$$

Derivation of Symplectic Lanczos Algorithm via J-Tridiagonalization

Compute (permuted) J-tridiagonal form of a (permuted) Hamiltonian matrix H (H_P) by column-wise evaluation of $HS = S\widetilde{H}$ ($H_P S_P = S_P \widetilde{H}_P$, where $S_P = [v_1, w_1, v_2, w_2, \ldots, v_n, w_n]$ is a permuted symplectic matrix). $\Longrightarrow$

$$H_P v_m = \delta_m v_m + \nu_m w_m$$

$$\Longleftrightarrow \quad \nu_m w_m = H_P v_m - \delta_m v_m =: \widetilde{w}_m$$

$$H_P w_m = \zeta_m v_{m-1} + \beta_m v_m - \delta_m w_m + \zeta_{m+1} v_{m+1}$$

$$\Longleftrightarrow \quad \zeta_{m+1} v_{m+1} = H_P w_m - \zeta_m v_{m-1} - \beta_m v_m + \delta_m w_m =: \widetilde{v}_{m+1}.$$

$\Longrightarrow$ Choose parameters $\delta_m, \beta_m, \nu_m, \zeta_m$ such that resulting algorithm computes J_P-orthogonal basis of Krylov subspace

$$\mathcal{K}(H_P, v_1, \ell) = \operatorname{span}\{v_1, H_P v_1, \ldots, H_P^{2\ell-1} v_1\}.$$

Choice of Parameters

Want $S_P^T J_P S_P = J_P \implies$

$$\nu_{m+1} = v_{m+1}^T J_P H_P v_{m+1}, \qquad \beta_m = -w_m^T J_P H_P w_m, .$$

$\zeta_m \neq 0, \delta_m$ are free!

$\zeta_m = ||\widetilde{v}_m||_2 \implies \|v_m\|_2 = 1$

Possible choices for δ_m:

$\delta_m = 1$ *[B./Faßbender '97]*

$\delta_m = v_m^T H_P v_m \implies v_m \perp w_m$ *[Lin/Ferng/Wang '97]*

$\delta_m = 0 \implies$ algorithm is equivalent to HR/HZ tridiagonalization

[B./Faßbender/Watkins '97, Watkins '02]

Generic Symplectic Lanczos Algorithm

Choose initial vector $\widetilde{v}_1 \in \mathbb{R}^{2n}$, $\widetilde{v}_1 \neq 0$.

$m = 1; \quad v_0 = 0; \quad \zeta_1 = ||\widetilde{v}_1||_2; \quad \nu_0 = 1$

while $\zeta_m \neq 0$ and $\nu_{m-1} \neq 0$

$\quad v_m = \widetilde{v}_m / \zeta_m$

$\quad \widetilde{w}_m = H_P v_m - \delta_m v_m$

$\quad \nu_m = v_m^T J_P H_P v_m$

$\quad$ **if** $\nu_m \neq 0$

$\quad$ **then** $w_m = \widetilde{w}_m / \nu_m$

$\qquad \beta_m = -w_m^T J_P H_P w_m$

$\qquad \widetilde{v}_{m+1} = H_P w_m - \zeta_m v_{m-1} - \beta_m v_m + \delta_m w_m$

$\qquad \zeta_{m+1} = ||\widetilde{v}_{m+1}||_2$

$\quad$ **end if**

$\quad m = m + 1$

end while

Lanczos Recursion and Breakdown

Define $S_P^{2k} = [v_1, w_1, v_2, w_2, \ldots, v_k, w_k] \in \mathbb{R}^{2n \times 2k}$, let $\widetilde{H}_P^{2k}$ be the leading $2k \times 2k$ principal submatrix of $\widetilde{H}_P$, then the symplectic Lanczos recursion is

$$H_P S_P^{2k} = S_P^{2k} \widetilde{M}_P^{2k} + \zeta_{k+1} v_{k+1} e_{2k}^T.$$

Breakdown is possible:

$\widetilde{v}_m = 0 \Rightarrow \zeta_m = 0$, symplectic invariant subspace of H is detected,
lucky breakdown!

$\widetilde{w}_m = 0 \Rightarrow \nu_m = 0$, invariant subspace of H_P of dimension $2m - 1$ is detected,
lucky breakdown!

$\nu_m = 0$ but $v_m \neq 0$ and $w_m \neq 0$
$\Longrightarrow$ serious breakdown!

Uniqueness of Lanczos Vectors

Theorem:

If there are two symplectic Lanczos recurrences with $v_1 = v_1$

$$HV_k = V_k H_k + \zeta_{k+1}\tilde{v}_{k+1}e_{2k}^T,$$
$$HV_k = V_k H_k + \zeta_{k+1}\tilde{v}_{k+1}e_{2k}^T,$$

then there exists a trivial symplectic matrix $D_k = \begin{bmatrix} \hat{D}_k & \hat{F}_k \\ & \hat{D}_k^{-1} \end{bmatrix}$, $\hat{D}_k, \hat{F}_k$ diagonal, such that $V_k = V_k D_k$.

Proof:

Consequence of uniqueness of SR decomposition up to trivial symplectic factors and relation of SR decomposition to Krylov subspace. □

Condition of Lanczos Basis

Accuracy of computed eigenvalues is affected by condition of Lanczos basis.

$\Rightarrow$ keep $\mathrm{cond}_2(V_n)$ small (i.e., choose "best" trivial symplectic factor D_k)

$$V_n \text{ symplectic} \quad \Longrightarrow \quad V_n^{-1} = -JV_n^T J \quad \Longrightarrow \quad \mathrm{cond}_2(V_n) = \|V_n\|_2^2.$$

$\|V_n\|_2$ can be bounded by

$$\max_{1\le k\le n}\{\|v_k\|_2, \|w_k\|_2\} \le \|V_n\|_2 \le \sqrt{2}n \max_{1\le k\le n}\{\|v_k\|_2, \|w_k\|_2\},$$

$\Longrightarrow$ Minimize $\tau := \max_{1\le k\le n}\{\|v_k\|_2, \|w_k\|_2\}$.

Optimizing One Free Parameter

Fix ζ_k such that $\|v_k\|_2 = 1$ for all $k \implies$

$$\tau = \max_{1\leq k\leq n}\{\|w_k\|_2\} = \max_{1\leq k\leq n}\{\frac{1}{|\nu_k|}\|Hv_k - \delta_k v_k\|_2\}.$$

Requiring symplectic Lanczos basis $\Rightarrow \nu_k$ is fixed.

Choice of δ_k independent of $\delta_1, \ldots, \delta_{k-1} \implies$

$$\delta_k = \operatorname*{argmin}_{\delta\in\mathbb{R}}\{\|Hv_k - \delta v_k\|_2\}.$$

Minimizing τ

Consider the quadratic form

$$\begin{aligned} f_k(\delta) &= \|Hv_k - \delta v_k\|_2^2 = (Hv_k - \delta v_k)^T (Hv_k - \delta v_k) \\ &= v_k^T H^T H v_k - 2\delta v_k^T H v_k + \delta^2 \underbrace{v_k^T v_k}_{=1}. \end{aligned}$$

First-order necessary condition for a minimum is

$$f_k'(\delta) = -2v_k^T H v_k + 2\delta = 0.$$

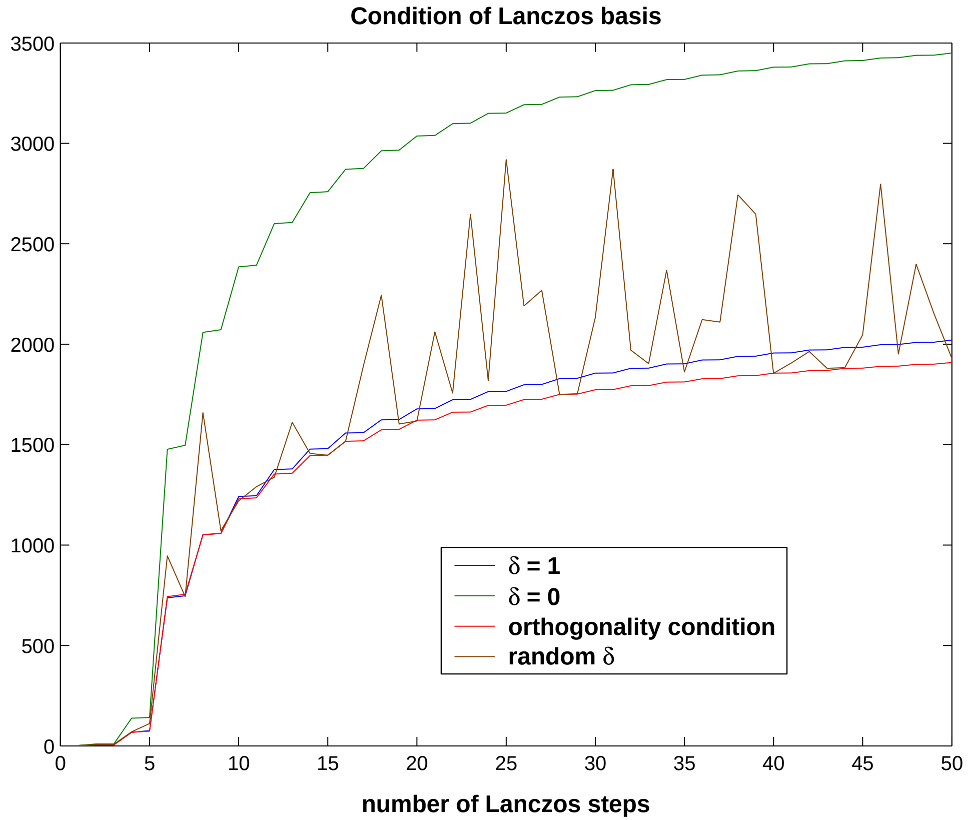
Hence,

$$\delta_k = v_k^T H v_k, \text{ i.e., } v_k \perp w_k \text{ (local orthogonality condition)}$$

$\Rightarrow$ Same choice as in [Ferng/Lin/Wang '97].

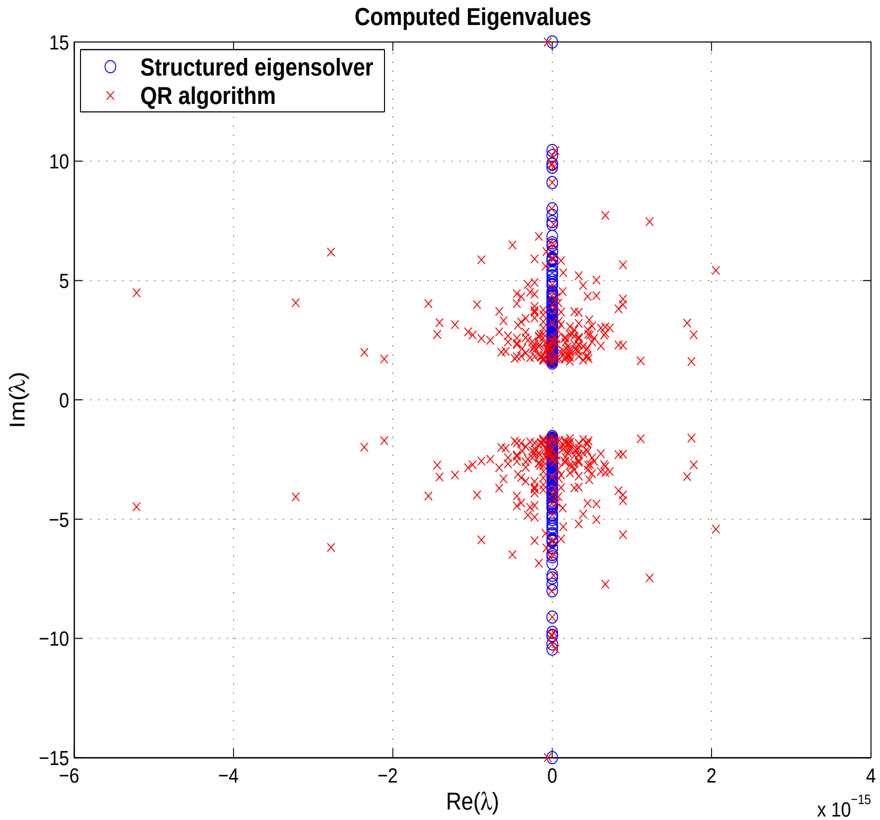
Numerical Examples I

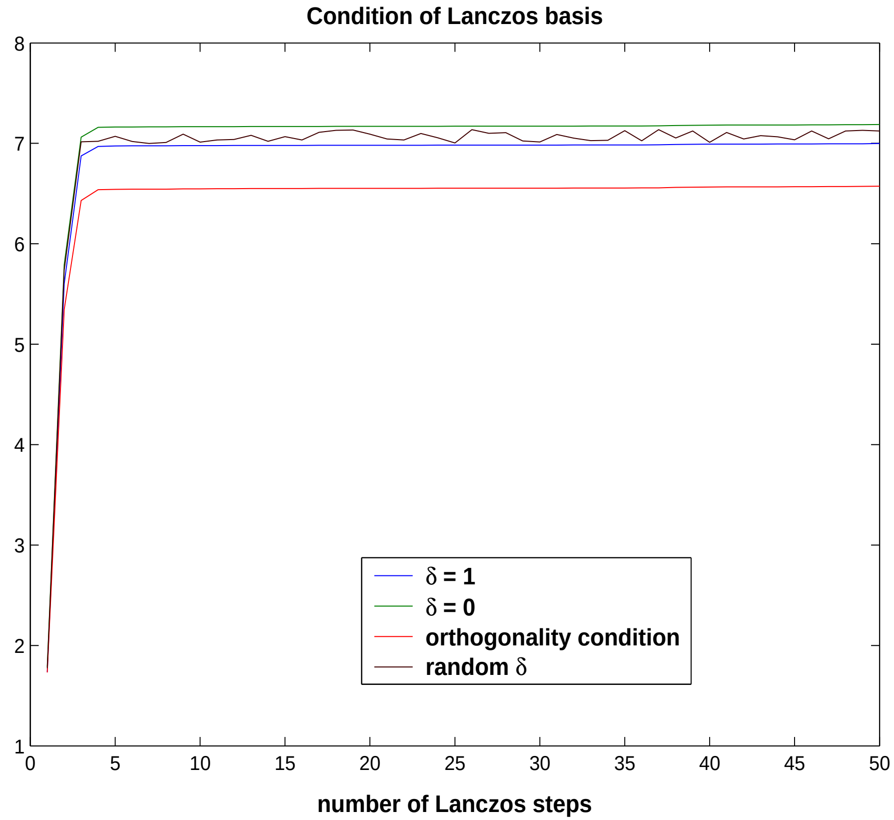
Control of string of high-speed vehicles: $n = 398$, $v = e$, different choices for δ_j



Numerical Examples II

Random stable gyroscopic system: $n = 200$, different choices for δ_j





Conclusions

- Optimal choice of free parameters in symplectic Lanczos method can improve condition of Lanczos basis and may improve Ritz value accuracy.

- Optimization of two free parameters possible but . . .

- Thorough comparison necessary.

- For practical applications, use implicitly restarted variants [B./Fassbender '97, Watkins '02], but still more details necessary: shift-and-invert, deflation, locking, purging, . . .

- Variants for symplectic eigenproblem available [B./Fassbender '00].

- Two-sided symplectic (implicitly restarted) Arnoldi based on symplectic URV decomposition under development [B./Kressner/Mehrmann/Xu].