# Structured Lanczos Algorithms for Quadratic Eigenproblems

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# Quadratic Eigenvalue Problems

Consider

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

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

Motivation:

- 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]

In these applications, usually $-K$ is spd.

# Properties

Spectrum of

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

has Hamiltonian symmetry:

$$\text{eigenvalues occur in} \left\{ \begin{array}{ll} \text{pairs} & (\lambda, -\lambda) \text{ if } \lambda \in \mathbb{R}, i\mathbb{R} \\ \text{quadruples} & (\lambda, \overline{\lambda}, -\lambda, -\overline{\lambda}) \end{array} \right. .$$

Linearize using $y = \lambda x$

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

$H = \left[\begin{smallmatrix} 0 & -K \\ M & 0 \end{smallmatrix}\right]$ is Hamiltonian: $(HJ)^T = HJ$

$N = \left[\begin{smallmatrix} M & G \\ 0 & M \end{smallmatrix}\right]$ is skew-Hamiltonian: $(NJ)^T = -NJ$

where

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

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

# Reformulation of $H - \lambda N$

Note:

$$N = Z_1 Z_2 = \begin{bmatrix} I & \frac{1}{2}G \\ 0 & M \end{bmatrix} \begin{bmatrix} M & \frac{1}{2}G \\ 0 & I \end{bmatrix}.$$

Hence as $M$ spd

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

where

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

$W$ is Hamiltonian!

$\Longrightarrow$ eigenvalues occur in $\begin{cases} (\lambda, -\lambda) \text{ if } \lambda \in \mathbb{R}, i\mathbb{R} \\ (\lambda, \overline{\lambda}, -\lambda, -\overline{\lambda}) \end{cases}.$

# Shift-and-Invert

Problem: Find eigenvalues of $W$ nearest to $\lambda_0$.

Standard approach: consider $(W - \lambda_0 I)^{-1}$

destroys structure! $\Rightarrow$ no eigenvalue pairing

Remedy: use $\begin{cases} (\lambda_0, -\lambda_0) \text{ if } \lambda_0 \in \mathbb{R}, i\mathbb{R} \\ (\lambda_0, \overline{\lambda_0}, -\lambda_0, -\overline{\lambda_0}) \text{ if } \lambda_0 \in \mathbb{C} \end{cases}$.

E.g., for $\lambda_0 \in \mathbb{R}, i\mathbb{R}$

$$R_2(\lambda_0) = (W - \lambda_0 I)^{-1}(W + \lambda_0 I)^{-1}$$

or for $\lambda_0 \in \mathbb{C}$

$$R_4(\lambda_0) = R_2(\lambda_0) R_2(\overline{\lambda_0})$$

$R_2(\lambda_0), R_4(\lambda_0)$ are real skew-Hamiltonian.

$\Rightarrow$ apply skew-Hamiltonian implicitly restarted Arnoldi iteration (SHIRA) [Mehrmann/Watkins '00]

## Other possibilities:

**use (generalized) Cayley-transformation**

For $\lambda_0 \in \mathbb{R}$

$$M_2(\lambda_0) = (W - \lambda_0 I)^{-1}(W + \lambda_0 I)$$

or for $\lambda_0 \in \mathbb{C}$

$$M_4(\lambda_0) = M_2(\lambda_0) M_2(\overline{\lambda_0})$$

$\Longrightarrow M_2(\lambda_0), M_4(\lambda_0)$ are real symplectic.

$M \in \mathbb{R}^{2n \times 2n}$ symplectic

$$\Updownarrow$$

$$M^T J M = J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$$

- Lie group
  $\Longrightarrow M^{-1} = -JM^T J.$
  $\Longrightarrow$ If $S$ symplectic, then $S^{-1}MS$ symplectic.
- $\lambda \in \sigma(M) \Longrightarrow \overline{\lambda^{-1}} \in \sigma(M).$
  $\lambda \in \mathbb{R} \Longrightarrow \lambda^{-1} \in \sigma(M).$
  $\lambda \in \mathbb{C} \Longrightarrow \overline{\lambda}, \lambda^{-1}, \overline{\lambda^{-1}} \in \sigma(M).$

$\Rightarrow$ apply implicitly restarted symplectic Lanczos iteration [B./Fassbender '98]

**keep Hamiltonian structure**

For $\lambda_0 \in \mathbb{R}, i\mathbb{R}$

$$W_2(\lambda_0) = (W - \lambda_0 I)^{-1}(W + \lambda_0 I)^{-1} W^{-1}$$

or $\lambda_0 \in \mathbb{C}$

$$W_4(\lambda_0) = W_2(\lambda_0) W_2(\overline{\lambda_0}) W$$

$\Longrightarrow$ $W_2(\lambda_0)$, $W_4(\lambda_0)$ are real Hamiltonian.

$$M \in \mathbb{R}^{2n \times 2n} \text{ Hamiltonian}$$
$$\Updownarrow$$
$$MJ = (MJ)^T$$

- Lie algebra
  $\Longrightarrow$ if $S$ symplectic, then $S^{-1}MS$ Hamiltonian.

$\Rightarrow$ apply implicitly restarted symplectic Lanczos iteration
[B./Fassbender '97, B./Fassbender/Watkins '01]

# The Hamiltonian $J$-Hessenberg Form

For every Hamiltonian matrix $M$ there exists symplectic similarity transformation $\widetilde{M} = S^{-1}MS$ where

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

Hamiltonian $J$-Hessenberg/$J$-triangular form

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

# Some Notation

$$\begin{aligned} M_P &:= PMP^T, \quad \widetilde{M}_P := P\widetilde{M}P^T, \\ S_P &:= PSP^T, \quad J_P := PJP^T \end{aligned}$$

with the permutation matrix

$$P := [e_1, e_3, \ldots, e_{2n-1}, e_2, e_4, \ldots, e_{2n}] \in \mathbb{R}^{2n\times 2n}.$$

From $S^TJS = J$ we obtain

$$S_P^T J_P S_P = J_P = \begin{bmatrix} 0 & 1 & & & \\ -1 & 0 & & & \\ & & \ddots & & \\ & & & 0 & 1 \\ & & & -1 & 0 \end{bmatrix},$$

while $S^{-1}MS = \widetilde{M}$ yields $S_P^{-1}M_PS_P = \widetilde{M}_P,$ where

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

# Symplectic Lanczos Algorithm

Aim: Lanczos-like method for computing $J$-Hessenberg form $S^{-1}MS = \widetilde{M}$ of a Hamiltonian matrix $M$. Permuted version

$$S_P^{-1} M_P S_P = \widetilde{M}_P.$$

Given $v_1$, let $S_P = [v_1, w_1, v_2, w_2, \ldots, v_n, w_n]$ be a permuted symplectic matrix. Computing $S_P$ in a Lanczos-like style columnwise from

$$M_P S_P e_j = S_P \widetilde{H}_P e_j, \qquad j = 1, 2, \ldots$$

we obtain for odd numbered columns

$$\begin{aligned} M_P v_{m+1} &= \delta_{m+1} v_{m+1} + \nu_{m+1} w_{m+1} \\ \Longleftrightarrow \quad \nu_{m+1} w_{m+1} &= M_P v_{m+1} - \delta_{m+1} v_{m+1} \end{aligned}$$

and for even numbered columns

$$\begin{aligned} M_P w_m &= \zeta_m v_{m-1} + \beta_m v_m - \delta_m w_m + \zeta_{m+1} v_{m+1} \\ \Longleftrightarrow \quad \zeta_{m+1} v_{m+1} &= M_P w_m - \zeta_m v_{m-1} - \beta_m v_m + \delta_m w_m \end{aligned}$$

$\Rightarrow$ Algorithm computes $J_P$-orthogonal basis of Krylov space

$$\mathcal{S}(M_P, s_1, \ell) = \{s_1, M_P s_1, \ldots, M_P^{2\ell-1} s_1\}.$$

# Choice of Parameters

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

$$\zeta_{m+1} = ||\widetilde{v}_{m+1}||_2, \quad \nu_{m+1} = v_{m+1}^T J_P M_P v_{m+1},$$

$$\beta_m = -w_m^T J_P M_P w_m, \qquad \delta_m \text{ is free!}$$

$\Longrightarrow$ *Symplectic Lanczos Method*

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 $\nu_{m-1} \neq 0$

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

$\widetilde{w}_m = M_P v_m - \delta_m v_m$

$\nu_m = v_m^T J_P M_P v_m$

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

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

$\beta_m = -w_m^T J_P M_P w_m$

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

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

**end if**

$m = m + 1$

**end while**

Possible choices for $\delta_m$:

$\delta_m = 1$ [*B./Faßbender '97*]

$\delta_m = v_m^T M_P v^m \Rightarrow v_m \perp w_m$ [*Lin/Ferng/Wang '97*]

$\delta_m = 0 \Rightarrow$ algorithm is equivalent to HZ tridiagonalization [*B./Faßbender/Watkins '01*]

# Lanczos Recursion and Breakdown

Define

$$S_P^{2k} = [v_1, w_1, v_2, w_2, \ldots, v_k, w_k] \in \mathbb{R}^{2n \times 2k}$$

and let $\widetilde{H}_P^{2k}$ be the leading $2k \times 2k$ principal submatrix of $\widetilde{M}_P$, then the Lanczos recursion is

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

Breakdown is possible:

$\widetilde{v}_{m+1} = 0 \Rightarrow \zeta_{m+1} = 0$, symplectic invariant subspace of $H$ is detected, lucky breakdown

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

$\nu_{m+1} = 0$ but $v_{m+1} \neq 0$ and $w_{m+1} \neq 0$
$\Longrightarrow$ serious breakdown

# Implicit Restarts

Assume that $S_P^{2k} \in \mathbb{R}^{2n \times 2k}$ is known with

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

For any permuted symplectic matrix $S_P \in \mathbb{R}^{2k \times 2k}$ :

$$M_P \underbrace{(S_P^{2k} S_P)}_{\hat{S}_P^{2k}} = \underbrace{(S_P^{2k} S_P)}_{\hat{S}_P^{2k}} \underbrace{(S_P^{-1} \widetilde{M}_P^{2k} S_P)}_{\hat{M}_P^{2k}} + \zeta_{k+1} v_{k+1} e_{2k}^T S_P$$

Thus,

$$(*) \qquad M_P \hat{S}_P^{2k} = \hat{S}_P^{2k} \hat{M}_P^{2k} + \zeta_{k+1} v_{k+1} e_{2k}^T S_P.$$

Obtain new Lanczos recursion from $(*)$ $\Longrightarrow$

- $\mathrm{colspace}({P^n}^T \hat{S}_P^{2k} P^k)$ must be symplectic,
- $\hat{M}_P^{2k}$ must have Hamiltonian $J$-Hessenberg form,
- the residual term $\zeta_{k+1} v_{k+1} e_{2k}^T S_P$ has to be of the form 'vector $\times$ $e_{2k}$'.

$\Longrightarrow$ (permuted) SR decomposition of
$p(\widetilde{M}^{2k}) = \widetilde{M}^{2k} - \mu I$ or other shift polynomial.

# A k-step Symplectic Lanczos Algorithm

Input: Hamiltonian matrix $H \in \mathbb{R}^{2n \times 2n}$;
vector $v_1 \in \mathbb{R}^{2n}$; integers $k$, $p$; tolerance $tol$.

Output: symplectic basis for $2k$–dimensional $H$–invariant subspace.

1. Compute $k$ steps of symplectic Lanczos method with initial vector $v_1$ such that

$$M_P S_P^{2k} = S_P^{2k}{}_P^{2k} + r_{k+1} e_{2k}^T.$$

2. $\zeta = \|r_{k+1}\|_2$
3. WHILE $\zeta > tol$ DO

   (a) Compute $p$ steps of symplectic Lanczos method such that

   $$M_P S_P^{2(k+p)} = S_P^{2(k+p)} \widetilde{M}_P^{2(k+p)} + r_{k+p+1} e_{2(k+p)}^T.$$

   (b) Choose $p$ shifts.

   (c) Implicitly restart the symplectic Lanczos method with the starting vector

   $$\hat{v}_1 = \rho(M_P - \mu_p I) \cdots (M_P - \mu_1 I) v_1$$

   via implicit single and double shift SR steps; obtain new Lanczos identity

   $$M_P \hat{S}_P^{2k} = \hat{S}_P^{2k} \hat{M}_P^{2k} + \hat{r}_{k+1} e_{2k}^T.$$

   (d) $\zeta = \|\hat{r}_{k+1}\|_2$

   END WHILE

END

# Applying the Operator

Recall: $\lambda^2 Mx + \lambda Gx + Kx = 0 \rightsquigarrow$

$$\Big(\underbrace{\begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & -K \\ M^{-1} & 0 \end{bmatrix} \begin{bmatrix} I & -\frac{1}{2}G \\ 0 & I \end{bmatrix}}_{=:W} - \lambda I\Big) \begin{bmatrix} y \\ x \end{bmatrix} = 0$$

Apply the shift-and-invert operator:

$$\begin{aligned} W_2(\lambda_0) &= (W - \lambda_0 I)^{-1}(W + \lambda_0 I)^{-1} W^{-1} \\ &= \begin{bmatrix} M & \lambda_0 M + \frac{1}{2}G \\ 0 & I \end{bmatrix} \\ &\quad \times \begin{bmatrix} 0 & I \\ -(\lambda_0^2 M + \lambda_0 G + K)^{-1} & 0 \end{bmatrix} \\ &\quad \times \begin{bmatrix} I & G \\ 0 & I \end{bmatrix} \begin{bmatrix} 0 & I \\ -(\lambda_0^2 M - \lambda_0 G + K)^{-1} & 0 \end{bmatrix} \\ &\quad \times \begin{bmatrix} I & G - \lambda_0 M \\ 0 & M \end{bmatrix} \times \begin{bmatrix} 0 & M \\ -K^{-1} & 0 \end{bmatrix} \\ &\quad \times \begin{bmatrix} I & \frac{1}{2}G \\ 0 & I \end{bmatrix} \end{aligned}$$

- Similar formulae for other operators.
- Need sparse factorizations of $\lambda_0^2 M \pm \lambda_0 G + K$, $K$.

# Where is CG in this talk?

If eigenvalues of largest magnitude are aim of computation $\Longrightarrow$ no shift-and-invert, just apply

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

Often $\lambda_0 = 0$ is suitable target shift $\Longrightarrow$

instead of $W_2(0)$ use

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

$M, K$ are spd $\Longrightarrow$ solve using CG!

# Concluding Remarks

- Application of $W_2(\lambda_0), W_4(\lambda_0)$ is more expensive than $M_2(\lambda_0), M_4(\lambda_0)$ or $R_2(\lambda_0), R_4(\lambda_0)$ due to additional factor $W^{-1}$ ($\rightsquigarrow$ additional application of $K^{-1}$ or $M^{-1}$).

  For $\lambda_0 = 0$, $W^{-1}$ is the cheapest operator!

- Preliminary numerical tests show similar convergence behavior for skew-Hamiltonian, Hamiltonian, symplectic operators.

  If $\lambda_0 = 0$ is suitable target shift, then $W^{-1}$ appears to be favorable.

- Advantage of Hamiltonian and symplectic approach: obtain eigenvectors directly!

  (skew-Hamiltonian case: $\pm\lambda \rightarrow \tilde{\lambda} \Longrightarrow$ obtain linear combinations of eigenvectors!)