Locking and Purging for the Hamiltonian Lanczos Process

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Basic definitions

Definition

A matrix S is symplectic $\iff S^T J S = J$ with $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$.

Definition

$$\text{A matrix } H \text{ is Hamiltonian} \iff (JH)^T = JH$$

$$\iff H = \begin{bmatrix} A & G \\ Q & -A^T \end{bmatrix}, \quad \begin{matrix} G = G^T \\ Q = Q^T \end{matrix}$$

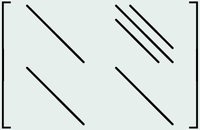
Properties

- If H is Hamiltonian and S is symplectic then $S^{-1}HS$ is Hamiltonian.
- If $\lambda \in \mathbb{R}$ is an eigenvalue of H then $-\lambda$ is also an eigenvalue of H.
- If $\lambda \in \mathbb{C}$ is an eigenvalue of H then $-\lambda, \bar{\lambda}, -\bar{\lambda}$ are also an eigenvalue of H.

Definition

A Hamiltonian J-Hessenberg matrix H is of the following structure

$H =$



SR decomposition

Definition

For $A \in \mathbb{R}^{2n,2n}$ is $A = SR$, the SR decomposition with a symplectic matrix S and a J-triangular matrix R.

- The SR decomposition is unique $\Rightarrow$ an equivalent to the implicit Q theorem holds.
- If H is a Hamiltonian J-Hessenberg matrix and p_k is a polynomial, then $S^{-1}HS$ is also a Hamiltonian J-Hessenberg matrix with S from the decomposition of $p_k(H) = SR$.

Implicit shifts

1. Single shift $(H - \mu I)$
2. Double shift $(H - \mu I)(H + \mu I)$
3. Quadrupel shift $(H - \mu I)(H + \bar{\mu} I)(H + \mu I)(H - \bar{\mu} I)$
    - Compute first column v
    - Compute transformation W such that $Wv = \alpha e_1$
    - Compute bulge chasing algorithm for $W^{-1}HW$

SR algorithm

SR algorithm

Perform implicit shifts until the permuted form H_p of the Hamiltonian J-Hessenberg matrix H is deflated and the blocks are of size 2×2 or 4×4.

$$H = \left[\begin{array}{ccc|ccc} \delta_1 & & & \beta_1 & \zeta_2 & \\ & \ddots & & \zeta_2 & \ddots & \\ & & \delta_n & & \zeta_n & \beta_n \\ \hline \nu_1 & & & -\delta_1 & & \\ & \ddots & & & \ddots & \\ & & \nu_n & & & -\delta_n \end{array}\right]$$

Eigenvalue and eigenvector computation

Eigenvalue computation

Only blocks of size 2×2 and 4×4 have to be considered. Explicit formulas for computing λ could be given.

Eigenvector computation

If $Re(\lambda) < 0$ easy eigenvector computation out of the SR algorithm by [Mehrmann/Bunse-Gerstner,1986].
If $Re(\lambda) > 0$ two ways for the eigenvector computation were developed

- Use inverse iteration with consideration of the sparse Hamiltonian structure.
- A Schur-like form could be used making advantage of the sparse Hamiltonian structure.

The symplectic Lanczos algorithm

- Use Lanczos recursion $H_p S_p^{2n,2k} = S_p^{2n,2k} \tilde{H}_p^{2k,2k} + \zeta_{k+1} v_{k+1} e_{2k}^T$
- Lanczos vectors $S_p^{2n,2k} = [v_1, w_1, v_2, w_2, \ldots, v_k, w_k]$ could be obtained
- Parameters of $\tilde{H}_p$ are computed

Symplectic Lanczos algorithm [Benner/Faßbender,1997]

1. $\delta_m = v_m^T H_p v_m$
2. $\tilde{w}_m = H_p v_m - \delta_m v_m$
3. $\nu_m = v_m^T J_p H_p v_m$
4. $w_m = \frac{1}{\nu_m} \tilde{w}_m$
5. $\beta_m = -w_m^T J_p H_p w_m$
6. $\tilde{v}_{m+1} = H_p w_m - \zeta_m v_{m-1} - \beta_m v_m + \delta_m w_m$
7. $\zeta_{m+1} = \|\tilde{v}_{m+1}\|_2$
8. $v_{m+1} = \frac{1}{\zeta_{m+1}} \tilde{v}_{m+1}$

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The implicitly restarted symplectic Lanczos algorithm

1. $H_p S_p^{2n,2m} = S_p^{2n,2m} \tilde{H}_p^{2m,2m} + \zeta_{m+1} v_{m+1} e_{2m}^T$
2. $(\tilde{H}_p^{2m} - \mu_i I)(\tilde{H}_p^{2m} + \mu_i I)(\tilde{H}_p^{2m} - \mu_{i+1} I)(\tilde{H}_p^{2m} + \mu_{i+1} I) = S_p^{(i)} R_p^{(i)}$
3. $H_p \check{S}_p^{2n,2m} = \check{S}_p^{2n,2m} \check{H}_p^{2m,2m} + \check{\zeta}_{m+1} \check{v}_{m+1} e_{2m}^T S_p$, with $\check{S}_p^{2n,2m} = S_p^{2n,2m} S_p$ and $\check{H}_p^{2m,2m} = S_p^{-1} \tilde{H}_p^{2m,2m} S_p$
4. Residual term

$$\zeta_{m+1} v_{m+1} (s_{2m,2m-4q} e_{2m-4q}^T + s_{2m,2m-3q} e_{2m-3q}^T + \ldots + s_{2m,2m} e_{2m}^T)$$

5. $H_p \check{S}_p^{2n,2k} = \check{S}_p^{2n,2k} \check{H}^{2k,2k} + r_k e_{2k}^T$
6. Residual $r_k = \check{\zeta}_{k+1} \check{v}_{k+1} + \zeta_{m+1} s_{2m,2k} v_{m+1}$

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Stopping criteria for IRSL

1. Assume $\tilde{H}^{2k,2k}$ could be diagonalized by usage of Y.
2. $HSY = SYY^{-1}\tilde{H}Y + \tilde{r}_k e_{2k}^T Y$ or $HX = X\Lambda + \tilde{r}_k e_{2k}^T Y$
3. Consider columns $Hx_i = -\lambda_i x_i + y_{2k,i}\tilde{r}_k$ and $Hx_{k+i} = \lambda_i x_{k+i} + y_{2k,k+i}\tilde{r}_k$
4. From the last equations we get eigentriples $(\lambda_i, x_{k+i}, (Jx_i)^T)$ and $(-\lambda_i, x_i, (Jx_{k+i})^T)$
5. From [Kahan/Parlett/Jiang,1982] backward error $\|E_{\lambda_i}\|$,where $(H - E_{\lambda_i})x = \lambda_i x$, could be computed

$$\|E_{\lambda_i}\| = \max\left\{\frac{|y_{2k,k+i}|\|\tilde{r}_k\|}{\|x_{k+i}\|}, \frac{|y_{2k,i}|\|\tilde{r}_k^T J\|}{\|Jx_i\|}\right\}.$$

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Krylov-Schur like decomposition

Krylov decomposition

Take $S_p^{2k} = (s_1, \ldots, s_{2k})$ with linear independent vectors s_j. A decomposition of the following structure $H_p S_p^{2k} = S_p^{2k} \tilde{H}_p^{2k} + s_{2k+1} \tilde{h}_{2k+1}^T$ is called *Krylov decomposition of order* $2k$.

Krylov-Schur like decomposition

Take $S_p^{2k} = (s_1, \ldots, s_{2k})$ with J-orthogonal vectors $s_j \Rightarrow$ $(S_p^{2k})^T J_p S_p^{2k} = J_p$ holds. A decomposition $H_p S_p^{2k} = S_p^{2k} \tilde{H}_p^{2k} + s_{2k+1} \tilde{h}_{2k+1}^T$ is called *Krylov-Schur like decomposition of order* $2k$, where $\tilde{H}_p^{2k}$ is a permuted Hamiltonian J-Hessenberg matrix in Schur form.

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Lanczos factorisation → Krylov-Schur like decomposition

1. Start with **Lanczos factorisation**

$$H_p S_p^{2n,2k} = S_p^{2n,2k} \tilde{H}_p^{2k,2k} + r_k e_{2k}^T.$$

2. Take S_p form SR algorithm to get $H_p S_p^{2n,2k} S_p = S_p^{2n,2k} S_p (S_p^{-1} \tilde{H}_p^{2k,2k} S_p) + r_k e_{2k}^T S_p$
3. Result is **Krylov-Schur like decompostion**

$$H_p \breve{S}_p^{2n,2k} = \breve{S}_p^{2n,2k} \breve{H}_p^{2k,2k} + r_k s_p^T$$

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Krylov-Schur like decomposition → Lanczos factorisation

1. Start with **Krylov-Schur like decomposition** $H_p S_p^{2k} = S_p^{2k} \tilde{H}_p^{2k} + s_{2k+1} \tilde{h}_{2k+1}^T$
2. Compute matrix Q_p (product of Givens matrices) such that $\tilde{h}_{2k+1}^T Q_p = \alpha e_{2k}^T$ multiplication with Q_p results in $H_p S_p^{2k} Q_p = \check{S}_p^{2k} \check{H}_p^{2k} + \alpha s_{2k+1} e_{2k}^T$.
3. Transform $\check{H}_p^{2k}$ to Hamiltonian J-Hessenberg form. Use rowwise variation of JHESS algorithm by [Mehrmann/Bunse-Gerstner]. Structure of $\alpha s_{2k+1} e_{2k}^T$ is preserved and the result is a **Lanczos factorisation** $H_p \check{S}_p^{2k} = \check{S}_p^{2k} \check{H}_p^{2k} + \check{s}_{2k+1} e_{2k}^T$.

Krylov-Schur like decomposition → Lanczos factorisation

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Exchanging eigenblocks

We have now a matrix $\check{H}_p^{2k}$ in block diagonal form. If we exchange the eigenblocks by using symplectic transformations we will be able to implement Purging and Locking. The permuted symplectic matrix $T_p(n)$ allows to exchange eigenblocks in $\check{H}_p^{2k}$.

$$T_p(n) = \begin{bmatrix} & & & & 1 \\ & & & -1 & \\ & & \cdot^{\cdot^{\cdot}} & & \\ & 1 & & & \\ -1 & & & & \end{bmatrix} \in \mathbb{R}^{2n,2n}.$$

Stopping Criteria for Krylov-Schur like algorithm

1. Assume $\breve{H}^{2k,2k}$ could be diagonalized by usage of Y.
2. $H\breve{S}Y = \breve{S}YY^{-1}\breve{H}Y + \breve{r}_k q^T Y$ or $HX = X\Lambda + \breve{r}_k q^T Y$
3. Consider columns $Hx_i = -\lambda_i x_i + \breve{r}_k q^T y_i$ and $Hx_{k+i} = \lambda_i x_{k+i} + \breve{r}_k q^T y_{k+i}$
4. From the last equations we get eigentriples $(\lambda_i, x_{k+i}, (Jx_i)^T)$ and $(-\lambda_i, x_i, (Jx_{k+i})^T)$
5. From [Kahan/Parlett/Jiang,1982] backward error $\|E_{\lambda_i}\|$,where $(H - E_{\lambda_i})x = \lambda_i x$, could be computed

$$\|E_{\lambda_i}\| = \max\left\{\frac{\|\breve{r}_k q^T y_{k+i}\|}{\|x_{k+i}\|}, \frac{\|\breve{r}_k^T q y_i^T J\|}{\|Jx_i\|}\right\}$$

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Locking

- For the **wanted** eigenvalue λ_i $\|E_{\lambda_i}\|$ is sufficiently small.
- The corresponding eigenblock in $\breve{H}_p^{2k,2k}$ has to be moved to the left upper corner of $\breve{H}_p^{2k,2k}$ using the T_p transformations.
- Accumulation of this transformations in $\breve{S}_p$ guarantees that the first columns of S_p are associated with λ_i.
- Shrink $\breve{H}_p$ such that the eigenblock for λ_i will not be involved in further computations.
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Purging

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- Accumulation of this transformations in $\breve{S}_p$ guarantees that the first columns of S_p are associated with λ_i.
- Shrink $\breve{H}_p$ such that the eigenblock for λ_i will not be involved in further computations.
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Krylov-Schur like algorithm

1. $H_p S_p^{2n,2m} = S_p^{2n,2m} \tilde{H}_p^{2m,2m} + \zeta_{m+1} v_{m+1} e_{2m}^T$.
2. Compute SR algorithm for $\tilde{H}_p$.
3. Transform Lanczos factorisation into Krylov-Schur like decomposition.
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Results of SR algorithm

Comparison of implemented SR algorithm and Matlab's eig routine for matrix H from CAREX (Example16) benchmark collection by [Benner/Laub/Mehrmann, 1995].

$$H = \left[\begin{array}{ccccc|ccccc}
-2 & 1 & & & 1 & 1 & & & & \\
1 & -2 & 1 & & & & 1 & & & \\
 & 1 & \ddots & \ddots & & & & \ddots & & \\
 & & \ddots & \ddots & 1 & & & & 1 & \\
1 & & & 1 & -2 & & & & & 1 \\
\hline
1 & & & & & -2 & 1 & & & 1 \\
 & 1 & & & & 1 & -2 & 1 & & \\
 & & \ddots & & & & 1 & \ddots & \ddots & \\
 & & & 1 & & & & \ddots & \ddots & 1 \\
 & & & & 1 & 1 & & & 1 & -2
\end{array}\right] \in \mathbb{R}^{2n,2n}$$

SR algorithm vs. Matlab's eig

eig	SR algorithm
-4.09007692547218	-4.09007692547218
-4.09007692547217	-4.09007692547217
-3.83317281079134	-3.83317281079134
-3.35764070604493	-3.35764070604493
-2.73657991827709	-2.73657991827709
-2.73657991827709	-2.73657991827702
-2.07265697232460	-2.07265697232467
-2.07265697232460	-2.07265697232460
-1.49292460661253	-1.49292460661264
-1.12803607263302	-1.12803607263302
-1.00907878741279	-1.00907878741279
-1.00000000000000	-1.00000000000000

- Example 16 of CAREX with size 24
- Maximal condition number for the SR algorithm is 51.75

Krylov-Schur for Quadratic Eigenvalue Problem

Consider the Quadratic Eigenvalue Problem (QEP)

$$(\lambda^2 M + \lambda G + K)u = 0$$

with matrices M, G and $K \in \mathbb{C}^{n,n}$. The special QEP where $M = M^T > 0$, $G = -G^T$ und $-K = -K^T > 0$ has Hamiltonian distribution of the eigenvalues and can be transformed in a Hamiltonian eigenvalue problem. See [Apel/Mehrmann/Watkins,2002] or [Mehrmann/Watkins,2001]. The result is the matrix H of the following form

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

Krylov-Schur like vs. SHIRA

Krylov-Schur like algorithm

eigenvalue	residual
-0.90592878885719	2.813e-16
-0.90634686034789	1.752e-16
-1.07560224930035	2.970e-16
-1.60332758476210	2.576e-15
-1.65786577098053	3.323e-15
-1.66121735256369	2.576e-15

SHIRA algorithm

eigenvalue	residual
-0.90592878886122	6.945e-17
-0.90634686034999	1.325e-16
-1.07560224930036	3.933e-17
-1.60332758477172	1.639e-15
-1.65786577098970	6.311e-16
-1.66121735256372	2.157e-16

- Both algorithms need 3 iterations to reach convergence bound of 10^{-8}
- SR algorithm has maximal condition number of 21178
- Size of matrices M, G and K is $n = 5139$

Krylov-Schur like vs. Matlab's eigs

Krylov-Schur like algorithm

Eigenwerte	Residuen
-0.90592878885661	3.244e-16
-0.90634686034754	2.242e-16
-1.07560224930008	1.591e-16
-1.60332758476411	7.370e-16
-1.65786577098821	2.488e-15
-1.66121735257659	1.169e-14
-1.75605775398702	2.057e-15

Matlab's eigs routine

Eigenwerte	Residuen
-0.90592878886324	1.864e-16
-0.90634686035071	1.648e-16
-1.07560224930012	1.823e-16
-1.60332758476362	5.733e-17
-1.65786577099183	5.241e-15
-1.66121735256949	3.922e-15
-1.75605775408379	9.367e-14

- Matlab's eigs needs 11 iteration steps and the Krylov-Schur like algorithm 8 (convergence bound of 10^{-10} for both)
- Maximal condition number during Krylov-Schur like is 2518
- Size of matrices M, G and K is again $n = 5139$

1. Fortran or C implementation of the SR algorithm and the Krylov-Schur Process
2. Time measurement when comparing these algorithms with SHIRA, eig and eigs
3. Integration of more computable examples such as Positive-Real-Balancing or special QEPs