Locking and Purging for the Hamiltonian Lanczos Process

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Basic definitions

Definition

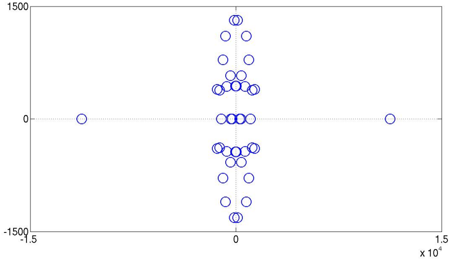
A matrix S is symplectic $\iff S^T J S = J$ with $J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix}$.

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.



SR algorithm

- SR algorithm by [Mehrmann/Bunse-Gerstner],[Della Dora] uses the SR decomposition
- Computes implicit shifts until permuted Hamiltonian J-Hessenberg matrix is deflated such that blocks are of size (2×2) or (4×4)

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

The symplectic Lanczos algorithm

- Use Lanczos recursion $H_p S_p^{2k} = S_p^{2k} \tilde{H}_p^{2k} + \zeta_{k+1} v_{k+1} e_{2k}^T$
- Lanczos vectors $S_p^{2k} = [v_1, w_1, v_2, w_2, \ldots, v_k, w_k]$ 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. $H_p S_p^{2m} = S_p^{2m} \tilde{H}_p^{2m} + \zeta_{m+1} v_{m+1} e_{2m}^T$
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. $H_p \check{S}_p^{2m} = \check{S}_p^{2m} \check{H}_p^{2m} + \check{\zeta}_{m+1} \check{v}_{m+1} e_{2m}^T S_p$, with $\check{S}_p^{2m} = S_p^{2m} S_p$ and $\check{H}_p^{2m} = S_p^{-1} \tilde{H}_p^{2m} S_p$
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. $H_p \check{S}_p^{2k} = \check{S}_p^{2k} \check{H}^{2k} + r_k e_{2k}^T$
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Why Purging and Locking?

- Gain efficiency because exclude unwanted but converged eigenvalues.
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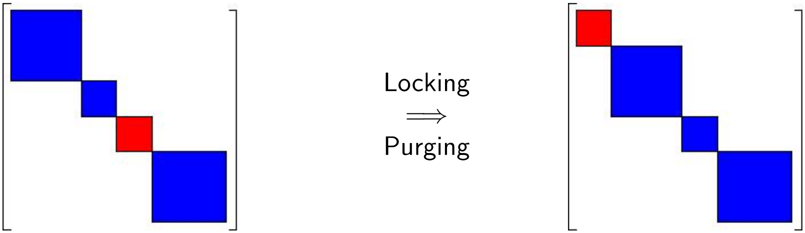
- Gain convergence speed by smaller matrices.



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 decomposition**

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

where $\check{S}_p = S_p^{2n,2k} S_p, \check{H}_p^{2k,2k} = (S_p^{-1} \tilde{H}_p^{2k,2k} S_p)$ and $s_p^T = e_{2k}^T S_p$.

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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 symplectic Givens matrices) such that $\tilde{h}_{2k+1}^T Q_p = \alpha e_{2k}^T$ multiplication with Q_p results in $H_p S_p^{2k} Q_p = \bar{S}_p^{2k} \bar{H}_p^{2k} + \alpha s_{2k+1} e_{2k}^T$.
3. Transform $\bar{H}_p^{2k}$ 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** $H_p \check{S}_p^{2k} = \check{S}_p^{2k} \check{H}_p^{2k} + \check{s}_{2k+1} e_{2k}^T$.

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Exchanging eigenblocks

- We have $\check{H}_p^{2k}$ in block diagonal form.
- Purging and Locking means exchanging eigenblocks in $\check{H}_p^{2k}$
- $T_p(j)$ is a permuted symplectic transformation which can exchange eigenblock

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

Stopping Criteria for Krylov-Schur like algorithm

1. Assume $\check{H}^{2k,2k}$ can be diagonalized by usage of Y.
2. $H\check{S}Y = \check{S}YY^{-1}\check{H}Y + \check{r}_k q^T Y$ or $HX = X\Lambda + \check{r}_k q^T Y$
3. Consider columns $Hx_i = -\lambda_i x_i + \check{r}_k q^T y_i$ and $Hx_{k+i} = \lambda_i x_{k+i} + \check{r}_k q^T y_{k+i}$
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 $(H - E_{\lambda_i})x = \lambda_i x$, can be computed

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

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3. Consider columns $Hx_i = -\lambda_i x_i + \check{r}_k q^T y_i$ and $Hx_{k+i} = \lambda_i x_{k+i} + \check{r}_k q^T y_{k+i}$
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 $(H - E_{\lambda_i})x = \lambda_i x$, can be computed

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

Stopping Criteria for Krylov-Schur like algorithm

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Locking

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

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- The corresponding eigenblock in $\check{H}_p^{2k,2k}$ has to be moved to the left upper corner of $\check{H}_p^{2k,2k}$ using the T_p transformations.
- Accumulation of this transformations guarantees that the first columns of $\check{S}_p$ are associated with λ_i.
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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. Apply SR algorithm to $\tilde{H}_p$.
3. Transform Lanczos factorisation into Krylov-Schur like decomposition.
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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 the SHIRA paper [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} with Shift $\sigma = 1$
- 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

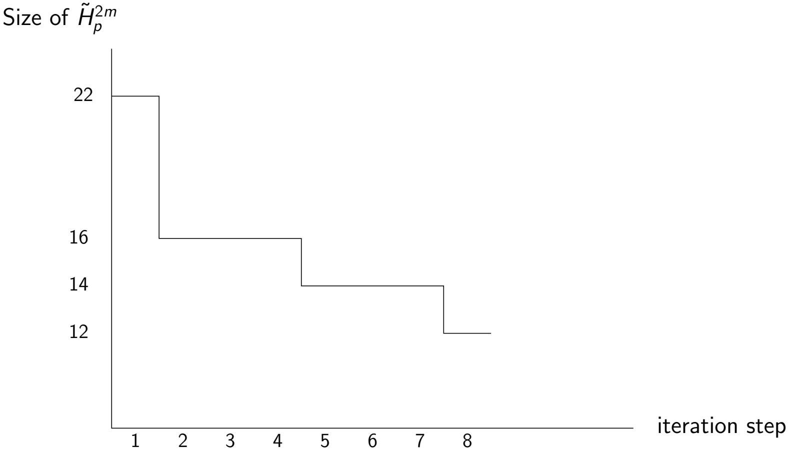
eigenvalue	residual
-0.90592878885661	3.244e-16
-0.90634686034754	2.242e-16
-1.07560224930008	1.591e-16
-1.60332758476411	7.370e-16
-1.65786577098821	2.488e-15
-1.66121735257659	1.169e-14
-1.75605775398702	2.057e-15

Matlab's eigs routine

eigenvalue	residual
-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 $n = 5139$

Gaining efficency



1. Fortran or C implementation of the SR algorithm and the Krylov-Schur Process
2. Time measurement when comparing these algorithms with SHIRA and eigs
3. Numerical results for more applications such as Positive-Real-Balancing or special QEPs
4. Transformation Q_p in the process of making a Lanczos factorisation out of a Krylov-Schur like decomposition such that $Q_p^{-1}\tilde{H}_p^{2m}Q_p$ has sparse structure.

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