SYMPLECTIC LANCOZS METHOD FOR SOLVING HAMILTONIAN SYSTEMS

1. Problem

Let's consider the linear Hamiltonain IVP:

$$\begin{aligned} \dot{y} &= Ay \\ y(0) &= y_0, \end{aligned} \tag{1.1}$$

where $A \in R^{2m,2m}$ is a Hamiltonian matrix, which means JA is a symmetric matrix. The energy for system (1.1) can be expresed as

$$\mathcal{H}_0(y) = \frac{1}{2} y^T JAy, \tag{1.2}$$

and $\mathcal{H}_0(y) \equiv \frac{1}{2} y_0^T JAy_0$.

Suppose $\hat{y} = y - y_0$, then the above equation (1.1) can be written as a linear Hamiltonian system with zero initial value as following:

$$\begin{aligned} \dot{\hat{y}} &= A\hat{y} + b, \\ \hat{y}(0) &= 0, \end{aligned} \tag{1.3}$$

where $b = Ay_0$. The energy for system (1.3) can be expressed as

$$\mathcal{H}_1(\hat{y}) = \frac{1}{2} \hat{y}^T JA\hat{y} + \hat{y}^T Jb, \tag{1.4}$$

and $\mathcal{H}_1(\hat{y}) \equiv 0$.

For coninence, we always use y for $\hat{y}$ in short in the following, namely we always consider system (1.3).

2. Symplectic Lancozs method for the Problem

The construction of the symplectic Lancozs method is based on the factorization of a Hamiltonian matrix which will be described in the following theorem.

Theorem 2.1 (Existence Theorem [1]). *If all leading principal minors of even dimension of $K[A, v_1, 2m]^T JK[A, v_1, 2m]$ are nonzero, then there exists a symplectic matrix $S^{2m,2m}$ with $Se_1 = v_1$ such that $H = (S^{2m,2m})^{-1} AS^{2m,2m}$ is an unreduced J-tridiagonal matrix.*

Here $K[A, v_1, 2m]^T JK[A, v_1, 2m]$ is the Krylov subspace generated based on matrix A and vector v_1.

Given a starting vector $v_1 \in R^{2m}$, the symplectic Lancozs method generates a sequence of matrices

$$S^{2m,2n} = [v_1, ..., v_n, w_1, ...w_n], \tag{2.1}$$

which satisfy

$$AS^{2m,2n} = S^{2m,2n} H^{2n,2n} + r_{n+1} e_{2n}^T. \tag{2.2}$$

In (2.2), $H^{2n,2n}$ is a tridiagnal Hamiltonian matrix

$$H^{2n,2n} = \begin{bmatrix} \mathrm{diag}([\delta_j]_{j=1}^n) & \mathrm{tridiag}([\zeta_j]_{j=2}^n, [\beta_j]_{j=1}^n, [\zeta_j]_{j=2}^n) \\ \mathrm{diag}([\nu_j]_{j=1}^n) & \mathrm{diag}([-\delta_j]_{j=1}^n) \end{bmatrix}, \tag{2.3}$$

$S^{2m,2n}$ is a symplectic matrx

$$S^{2m,2n^T} J^m S^{2m,2n} = J^n, \tag{2.4}$$

and the residual vector r_{n+1}, which is equal to $\zeta_{n+1} v_{n+1}$, is J-orthognal to the columns of $S^{2m,2n}$.

Now we consider applying the symplectic Lancozs method to system (1.3). Let b be the starting vector $v_1^{(1)}$ for generating the $2m \times 2m$ symplectic matrix $S^{(1)}$, namely we have $AS^{(1)} = S^{(1)} H^{(1)}$ and let $Z = [Z_1, ..., Z_{2m}] \in \mathbb{R}^{2m}$ be the vector that satisy $y = S^{(1)} Z$. We then can rewrite equation (1.3) as

$$\begin{aligned} S^{(1)} \dot{Z} &= AS^{(1)} Z + b, \\ Z(0) &= 0. \end{aligned} \tag{2.5}$$

Denote the $2m \times 2n$ symplectic matrix generated by symplectic Lancozs method with starting vector b as $S_n^{(1)}$, namely we have $AS_n^{(1)} = S_n^{(1)} H_n^{(1)} + r_{n+1}^{(1)} e_{2n}^T$. We approximate y with $S_n^{(1)} z$, where $z = [z_1, ..., z_{2n}] \in \mathbb{R}^{2n}$. Then we can consider

$$\begin{aligned} S_n^{(1)} \dot{z} &= AS_n^{(1)} z + b, \\ S_n^{(1)} z(0) &= 0. \end{aligned} \tag{2.6}$$

Multiplying equation (2.6) by $(J^n)^{-1} {S_n^{(1)}}^T J^m$ and denoting $(J^n)^{-1} {S_n^{(1)}}^T J^m b$ as $\tilde{b}$ gives

$$\begin{aligned} \dot{z} &= H_n^{(1)} z + \tilde{b}, \\ z(0) &= 0. \end{aligned} \tag{2.7}$$

Systerm (2.7) is also a Hamiltonian problem with energy

$$\mathcal{H}_2(z) = \frac{1}{2} z^T J^n H_n^{(1)} z + z^T J^n \tilde{b}, \tag{2.8}$$

and $\mathcal{H}_2(z) \equiv 0$.

By solving equation (2.7), we get an approximation for the solution of the original equation (1.1): $y_{[n]} = S_n^{(1)} z$. Now we will show that when we apply the symplectic Lanczos method to system (1.3), the energy will be preserved.

The numerical energy for symplectic Lanczos method is $\mathcal{H}_1(y_{[n]})$, and we observe

$$\begin{aligned}\mathcal{H}_1(y_{[n]}) &= \frac{1}{2} z^T {S_n^{(1)}}^T J A S_n^{(1)} z + z^T {S_n^{(1)}}^T J b, \\ &= \frac{1}{2} z^T {S_n^{(1)}}^T J (S_n^{(1)} H_n^{(1)} + r_{n+1} e_{2n}^T) + z^T {S_n^{(1)}}^T J b \\ &= \frac{1}{2} z^T J^n H_n^{(1)} z + z^T {S_n^{(1)}}^T J^n b \\ &= \mathcal{H}_2(z) \\ &= 0 \\ &= \mathcal{H}_1(y).\end{aligned} \tag{2.9}$$

3. Symplectic Lanczos method with resart

Denote the numerical error for symplectic Lanczos method as $\varepsilon^{(1)}$, namely $\varepsilon^{(1)} = y - S_n^{(1)} z$. From equation (1.3) and equation (2.7), we can get

$$\begin{aligned}&\dot{\varepsilon}^{(1)} = Ay - S_n^{(1)} H_n^{(1)} z + b - {S_n^{(1)}}^T \tilde{b} \\ &\varepsilon^{(1)}(0) = 0,\end{aligned} \tag{3.1}$$

Based on equation (2.2), we can replace $S_n^{(1)} H^{(1)}$ with $A S_n^{(1)} - r_{n+1} e_{2n}^T$. We then get an equation for the numerical error

$$\begin{aligned}&\dot{\varepsilon}^{(1)} = A \varepsilon^{(1)} + r_{n+1}^{(1)} e_{2n}^T z, \\ &\varepsilon^{(1)}(0) = 0.\end{aligned} \tag{3.2}$$

Systerm (3.2) is a non-autonomuns Hamiltonian system with energy

$$\mathcal{H}_3(t) = \frac{1}{2} {\varepsilon^{(1)}}^T J^m A \varepsilon^{(1)} + {\varepsilon^{(1)}}^T J^m r_{n+1} e_{2n}^T z(t) \tag{3.3}$$

We can also perform the symplectic Lanczos method to the error equation (3.2) and this is the basic idea for restart symplectic Lanczos method. Let v_{n+1} be the new starting vector $v_1^{(2)}$ for generating the new $2m \times 2m$ symplectic matrix S^2, which satisfy $AS^{(2)} = S^{(2)} H^{(2)}$, and $2m \times 2n$ symplectic matrix S_n^2 which satisfy $A S_n^{(2)} = S_n^{(2)} H_n^{(2)} + r_{n+1}^{(2)} e_{2n}^T$. We then can find $\Delta^{(1)}$ such that $\varepsilon^{(1)} = S^2 \Delta^{(1)}$ and let $\varepsilon^{(1)} \approx S_n^{(2)} \delta^{(1)} =$

$\varepsilon_{[n]}^{(1)}$, where

$$\begin{aligned}&\Delta_i^{(1)} = \delta_i^{(1)},\\ &\Delta_{m+i}^{(1)} = \delta_{n+i}^{(1)}, i = 1, 2, ..., n.\end{aligned} \tag{3.4}$$

Similarly we have

$$\begin{aligned}&\dot{\delta}^{(1)} = H_n^{(2)}\delta^{(1)} + (J^n)^{-1}{S_n^2}^T J^m r_{n+1}^{(2)} e_{2n}^T z\\ &\delta^{(1)}(0) = 0,\end{aligned} \tag{3.5}$$

Systerm (3.5) is a non-autonomuns Hamiltonian system with energy

$$\mathcal{H}_4(t) = \frac{1}{2}{\delta^{(1)}}^T J^n H_n^{(2)}\delta^{(1)} + {\delta^{(1)}}^T {S_n^2}^T J^m r_{n+1}^{(2)} e_{2n}^T z(t). \tag{3.6}$$

4. Analysis for the Energy of Error Equation

The exact solution for equation (1.3) can be written as $y = y_{[n]} + \varepsilon^{(1)}$. Thus we have (this is just normal calculation)

$$\begin{aligned}0 = \mathcal{H}_1(y) &= \frac{1}{2}(y_{[n]} + \varepsilon^{(1)})^T JA(y_{[n]} + \varepsilon^{(1)}) + (y_{[n]} + \varepsilon^{(1)})^T Jb,\\ &= \frac{1}{2}y_{[n]}^T JAy_{[n]} + {\varepsilon^{(1)}}^T JAy_{[n]} + \frac{1}{2}{\varepsilon^{(1)}}^T JA\varepsilon^{(1)} + y_{[n]}^T Jb + {\varepsilon^{(1)}}^T Jb\\ &= \frac{1}{2}y_{[n]}^T JAy_{[n]} + y_{[n]}^T Jb + {\varepsilon^{(1)}}^T JAy_{[n]} + {\varepsilon^{(1)}}^T Jb + \frac{1}{2}{\varepsilon^{(1)}}^T JA\varepsilon^{(1)}\\ &= \mathcal{H}_1(y_{[n]}) + {\varepsilon^{(1)}}^T JAS_n^{(1)} z + {\varepsilon^{(1)}}^T Jb + \frac{1}{2}{\varepsilon^{(1)}}^T JA\varepsilon^{(1)}\\ &= 0 + {\varepsilon^{(1)}}^T JAS_n^{(1)} z + {\varepsilon^{(1)}}^T Jb + \frac{1}{2}{\varepsilon^{(1)}}^T JA\varepsilon^{(1)}\\ &= {\varepsilon^{(1)}}^T JS_n^{(1)} H_n^{(1)} z + {\varepsilon^{(1)}}^T Jb + {\varepsilon^{(1)}}^T Jr_{n+1}e_{2n}^T z + \frac{1}{2}{\varepsilon^{(1)}}^T JA\varepsilon^{(1)}\\ &= {\varepsilon^{(1)}}^T JS_n^{(1)} H_n^{(1)} z + {\varepsilon^{(1)}}^T JS_n^{(1)} e_1 + \mathcal{H}_3(t)\\ &= {\varepsilon^{(1)}}^T JS_n^{(1)}\dot{z} + \mathcal{H}_3(t).\end{aligned} \tag{4.1}$$

Next we want to show that $\mathcal{H}_3(t) \equiv 0$ (The key point is to show the error term $\varepsilon^{(1)}$ is J orthognal to the columns of the matrix $S_n^{(1)}$. The skill here is to use $\varepsilon^{(1)} = S^{(1)}Z - S_n^{(1)}z$). Based on the construction of symplectic Lanczozs method, we can have

$${S^{(1)}}^T J^n S_n^{(1)} = \tilde{J}^{2m,2n}, \tag{4.2}$$

where

$$\tilde{J}^{2m,2n} = \begin{bmatrix} 0^{n,n} & I^{n,n} \\ 0^{m-n,n} & 0^{m-n,n} \\ -I^{n,n} & 0^{n,n} \\ 0^{m-n,n} & 0^{m-n,n} \end{bmatrix}, \tag{4.3}$$

and

$$\begin{aligned} Z_i &= z_i, \\ Z_{m+i} &= z_{n+i}, i = 1, 2, ..., n. \end{aligned} \tag{4.4}$$

Thus,

$$\begin{aligned} \varepsilon^{(1)^T} J S_n^{(1)} &= (S^{(1)} Z - S_n^{(1)} z)^T J S_n^{(1)} \\ &= Z^T \tilde{J}^{2m,2n} - z^T J^n \\ &= [-Z_{m+1}, ..., -Z_{m+n}, Z_1, ..., Z_n] - z^T J^n \\ &= 0. \end{aligned} \tag{4.5}$$

Equation (4.5) shows that the error term is J-orthognal to $S^{2n,2k}$. From equation (5.1) and (4.5) we get

$$\mathcal{H}_3(t) \equiv 0. \tag{4.6}$$

The above results (4.6) shows that the non-autonomuns Hamiltonian system (3.2) has in fact a constant enenrgy.

Denote the $2m \times 2(m-n)$ matrix $[v_{n+1}^{(2)}, ..., v_m^{(2)}, w_{n+1}^{(2)}, ..., w_m^{(2)}]$ as $S_{n-m}^{(2)}$ and the $2(m-n)$ vector $[\Delta_{n+1}^{(1)}, ..., \Delta_m^{(1)}, \Delta_{n+1}^{(1)}, ..., \Delta_m^{(1)}]^T$ as $\Delta_{2n-2k}^{(1)}$. The basic idea to prove $\mathcal{H}_4(t) \equiv 0$ is to see the difference between $\mathcal{H}_4(t)$ and $\mathcal{H}_3(t)$ is 0. It is easy to observe

$$\begin{aligned} \mathcal{H}_3(t) &= \frac{1}{2} \varepsilon^{(1)^T} J^m A \varepsilon^{(1)} + \varepsilon^{(1)^T} J^m r_{n+1} e_{2n}^T z(t) \\ &= \frac{1}{2} \varepsilon^{(1)^T} J^m A \varepsilon^{(1)} + (S^{(2)} \Delta^{(1)})^T J^m r_{n+1} e_{2n}^T z(t) \\ &= \frac{1}{2} \varepsilon^{(1)^T} J^m A \varepsilon^{(1)} + \Delta^{(1)^T} S^{(2)^T} J^m S^{(2)} e_1 e_{2n}^T z(t) \\ &= \frac{1}{2} \varepsilon^{(1)^T} J^m A \varepsilon^{(1)} - \delta_1^{(n+1)} z_{2n}, \end{aligned} \tag{4.7}$$

and

$$\begin{aligned} \mathcal{H}_4(t) &= \frac{1}{2} \delta^{(1)^T} J^n H_n^{(2)} \delta^{(1)} + \delta^{(1)^T} S_n^{2^T} J^m r_{n+1}^{(2)} e_{2n}^T z(t) \\ &= \frac{1}{2} \delta^{(1)^T} J^n H_n^{(2)} \delta^{(1)} + \delta^{(1)^T} S_n^{2^T} J^m S_n^2 e_1 e_{2n}^T z(t) \\ &= \frac{1}{2} \delta^{(1)^T} J^n H_n^{(2)} \delta^{(1)} - \delta_1^{(n+1)} z_{2n}, \end{aligned} \tag{4.8}$$

Thus we have

$$
\begin{aligned}
\frac{d}{dt}(\mathcal{H}_3(t)-\mathcal{H}_4(t)) &= \frac{d}{dt}(\frac{1}{2}\varepsilon^{(1)^T}J^mA\varepsilon^{(1)}-\frac{1}{2}\delta^{(1)^T}J^nH_n^{(2)}\delta^{(1)}) \\
&= \varepsilon^{(1)^T}J^mA\dot{\varepsilon}^{(1)}-\delta^{(1)^T}J^nH_n^{(2)}\dot{\delta}^{(1)} \\
&= \varepsilon^{(1)^T}J^mAr_{n+1}^{(1)}e_{2n}^Tz(t)-\delta^{(1)^T}J^nH_n^{(2)}e_1e_{2n}^Tz(t) \\
\\
&= (S_n^{(2)}\delta^{(1)}+S_{m-n}^{(2)}\Delta_{m-n}^{(1)})^TJ^mS_n^{(2)}e_1e_{2n}^Tz(t) \\
&- \delta^{(1)^T}J^nH_n^{(2)}e_1e_{2n}^Tz(t) \\
&= 0.
\end{aligned}
\tag{4.9}
$$

Equation (4.9) shows that $\mathcal{H}_4(t)\equiv\mathcal{H}_3(t)\equiv 0$.

5. Analysis for the Energy of Symplectic Lanczos method with restart

$$
\begin{aligned}
\mathcal{H}_1(y_{[n]}+\varepsilon_{[n]}^{(1)}) &= \frac{1}{2}(S_n^{(1)}z+S_n^{(2)}\delta^{(1)})^TJA(S_n^{(1)}z+S_n^{(2)}\delta^{(1)})+(S_n^{(1)}z+S_n^{(2)}\delta^{(1)})^TJb, \\
&= \frac{1}{2}z^TS_n^{(1)^T}JAS_n^{(1)}z+z^TS_n^{(1)^T}Jb+z^TS_n^{(1)^T}JAS_n^{(2)}\delta^{(1)} \\
&+ \frac{1}{2}\delta^{(1)^T}S_n^{(2)^T}JAS_n^{(2)}\delta^{(1)}+\delta^{(1)^T}S_n^{(2)^T}Jb, \\
&= H_1(y_{[n]})+z^TS_n^{(1)^T}JAS_n^{(2)}\delta^{(1)} \\
&+ \frac{1}{2}\delta^{(1)^T}S_n^{(2)^T}J(S_n^{(2)}H_n^{(2)}+r_{n+1}^{(2)}e_{2n}^T)\delta^{(1)}+\delta^{(1)^T}S_n^{(2)^T}JS_n^{(1)}e_1 \\
&= \frac{1}{2}\delta^{(1)^T}JH_n^{(2)}\delta^{(1)}+(S_n^{(2)}\delta^{(1)})^TJAS_n^{(1)}z+\delta^{(1)^T}S_n^{(2)^T}JS_n^{(1)}e_1 \\
&= \frac{1}{2}\delta^{(1)^T}JH_n^{(2)}\delta^{(1)}+(S_n^{(2)}\delta^{(1)})^TJ(S_n^{(1)}H_n^{(1)}+r_{n+1}^{(1)}e_{2n}^T)z \\
&+ \delta^{(1)^T}S_n^{(2)^T}JS_n^{(1)}e_1 \\
&= \mathcal{H}_4(t)+(S_n^{(2)}\delta^{(1)})^TJS_n^{(1)}\dot{z} \\
&= (S_n^{(2)}\delta^{(1)})^TJS_n^{(1)}\dot{z}.
\end{aligned}
\tag{5.1}
$$

References

[1] W. Ferng, W.-W. Lin, and C.-S. Wang, *The shift-inverted j-lanczos algorithm for the numerical solutions of large sparse algebraic riccati equations*, Computers & Mathematics with Applications, 33 (1997), pp. 23 – 40.