SYMPLECTIC LANCOZS METHOD FOR SOLVING HAMILTONIAN SYSTEMS

Let's consider the linear Hamiltonain IVP:

$$\begin{aligned} \dot{y} &= Ay \\ y(0) &= y_0, \end{aligned} \tag{0.1}$$

where $A \in R^{2n,2n}$ is a Hamiltonian matrix, namely JA is a symmetric matrix. The energy for system (0.1) can be expresed as

$$H_0(y) = \frac{1}{2} y^T JAy, \tag{0.2}$$

and $H_0(y) \equiv \frac{1}{2} y_0^T JAy_0$.

Suppose $\hat{y} = y - y_0$, then the above problem (0.1) can be written as a zero initial value linear Hamiltonian problem as following:

$$\begin{aligned} \dot{\hat{y}} &= A\hat{y} + b, \\ \hat{y}(0) &= 0, \end{aligned} \tag{0.3}$$

where $b = Ay_0$. The energy for system (0.3) can be expressed as

$$H_1(\hat{y}) = \frac{1}{2} \hat{y}^T JA\hat{y} + \hat{y}^T Jb, \tag{0.4}$$

and $H_1(\hat{y}) \equiv 0$.

For coninence, we always use y for $\hat{y}$ in short in the following.

1. Symplectic Lancozs method

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

$$S^{2n,2k} = [v_1, ..., v_k, w_1, ...w_k], \tag{1.1}$$

which satisfy

$$AS^{2n,2k} = S^{2n,2k} H_k^{2k,2k} + \zeta_{k+1} v_{k+1} e_{2k}^T. \tag{1.2}$$

In (1.2), $H_k^{2k,2k}$ is a tridiagnal Hamiltonian matrix

$$H_k^{2k,2k} = \begin{bmatrix} \operatorname{diag}([\delta_j]_{j=1}^k) & \operatorname{tridiag}([\zeta_j]_{j=2}^k, [\beta_j]_{j=1}^k, [\zeta_j]_{j=2}^k) \\ \operatorname{diag}([\nu_j]_{j=1}^k) & \operatorname{diag}([-\delta_j]_{j=1}^k) \end{bmatrix}, \tag{1.3}$$

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

$$S^{2n,2k^T} J^n S^{2n,2k} = J^k, \tag{1.4}$$

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

In fact, there is a strong theorem for the factorization of a Hamiltonian matrix.

Theorem 1.1 (Existence Theorem [1]). *If all leading principal minors of even dimension of $K[A, v_1, 2n]^T JK[A, v_1, 2n]$ are nonzero, then there exists a symplectic matrix $S^{2n,2n}$ with $Se_1 = v_1$ such that $H = (S^{2n,2n})^{-1}AS^{2n,2n}$ is an unreduced J-tridiagonal matrix.*

Here $K[A, v_1, 2n]^T JK[A, v_1, 2n]$ is the Krylov subspace generated based on matrix A and vector v_1. Let $v_1 = \frac{b}{\|b\|_2}$ be the starting vector for generating the symplectic matrix $S^{2n,2n}$ and let $Z = [Z_1, ..., Z_{2n}] \in \mathbb{R}^{2n}$ be the vector that satisy $y = S^{2n,2n}Z$. We can rewrite equation (0.3) as

$$\begin{aligned} &S^{2n,2n}\dot{Z} = AS^{2n,2n}Z + b,\\ &Z(0) = 0. \end{aligned} \tag{1.5}$$

Now we consider applying the symplectic Lanczos method to the system (0.3). Approximate y with $S^{2n,2k}z$, where $z = [z_1, ..., z_{2k}] \in \mathbb{R}^{2k}$. Then we can consider

$$\begin{aligned} &S^{2n,2k}\dot{z} = AS^{2n,2k}z + b,\\ &S^{2n,2k}z(0) = 0. \end{aligned} \tag{1.6}$$

Multiplying equation (1.6) by $(J^k)^{-1}S^{2n,2k^T}J^n$ gives

$$\begin{aligned} &\dot{z} = H_k^{2k,2k}z + (J^k)^{-1}S^{2n,2k^T}J^n b,\\ &z(0) = 0. \end{aligned} \tag{1.7}$$

Systerm (1.7) is also a Hamiltonian problem with energy

$$H_2(z) = \frac{1}{2}z^T J^k H_k^{2k,2k} z + z^T S^{2n,2k^T} J^n b, \tag{1.8}$$

and$H_2(z) \equiv 0$.

By solving equation (1.7), we get an approximation $y_{[k]} = S^{2n,2k}z$ for the solution of the original equation (0.1). Now we will show that when we apply the symplectic Lanczos method to system (0.3), the energy will be preserved.

We denote the numerical energy for symplectic Lanczos method as NH_1, then we have

$$
\begin{aligned}
NH_1(y_{[k]}) &= \frac{1}{2}z^T S^{2n,2k^T} JAS^{2n,2k}z + z^T S^{2n,2k^T} Jb, \\
&= \frac{1}{2}z^T S^{2n,2k^T} J(S^{2n,2k}H_k^{2k,2k} + \zeta_{k+1}v_{k+1}e_{2k}^T) + z^T S^{2n,2k^T} Jb \\
&= \frac{1}{2}z^T J^k H_k^{2k,2k} z + z^T S^{2n,2k^T} J^n b \\
&= H_2(z) \\
&= 0 \\
&= H_1(y).
\end{aligned}
\tag{1.9}
$$

2. Symplectic Lanczos method with resart

Denote the numerical error as ε, namely $\varepsilon = y - S^{2n,2k}z$. From equation (0.3) and equation (1.7), we can get

$$
\begin{aligned}
&\dot{\varepsilon} = Ay - S^{2n,2k}H_k^{2k,2k}z + b - (J^k)^{-1}S^{2n,2k^T}J^n b \\
&\varepsilon(0) = 0,
\end{aligned}
\tag{2.1}
$$

Based on equation (1.2), we can replace $S^{2n,2k}H_k^{2k,2k}$ with $AS^{2n,2k} - \zeta_{k+1}v_{k+1}e_{2k}^T$. We then get an equation for the numerical error

$$
\begin{aligned}
&\dot{\varepsilon} = A\varepsilon + \zeta_{k+1}v_{k+1}e_{2k}^T z, \\
&\varepsilon(0) = 0.
\end{aligned}
\tag{2.2}
$$

Systerm (2.2) is a non-autonomuns Hamiltonian system with energy

$$
H_3(t) = \frac{1}{2}\varepsilon^T J^n A\varepsilon + \varepsilon^T J^n \zeta_{k+1}v_{k+1}e_{2k}^T z(t) \tag{2.3}
$$

Let z be a starting vector $\tilde{v}_1$. We can perform the symplectic Lanczos method for the error equation (2.2). Suppose $\varepsilon \approx \tilde{S}^{2n,2m}\delta$, similarly we have

$$
\begin{aligned}
&\dot{\delta} = \tilde{H}^{2m,2m}\delta + (J^m)^{-1}S^{2n,2m^T}J^n\tilde{\zeta}_{k+1}\tilde{v}_{k+1}e_{2k}^T z \\
&\delta(0) = 0,
\end{aligned}
\tag{2.4}
$$

3. Analysis for the Energy of Error Equation

The exact solution for equation (0.3) can be written as $y = y_{[k]} + \varepsilon$. Thus we have

$$
\begin{aligned}
0 = H_1(y) &= \frac{1}{2}(y_{[k]} + \varepsilon)^T JA(y_{[k]} + \varepsilon) + (y_{[k]} + \varepsilon)^T Jb, \\
&= \frac{1}{2} y_{[k]}^T JAy_{[k]} + \varepsilon^T JAy_{[k]} + \frac{1}{2}\varepsilon^T JA\varepsilon + y_{[k]}^T Jb + \varepsilon^T Jb \\
&= \frac{1}{2} y_{[k]}^T JAy_{[k]} + y_{[k]}^T Jb + \varepsilon^T JAy_{[k]} + \varepsilon^T Jb + \frac{1}{2}\varepsilon^T JA\varepsilon \\
&= NH_1(y_{[k]}) + \varepsilon^T JAS^{2n,2k} z + \varepsilon^T Jb + \frac{1}{2}\varepsilon^T JA\varepsilon \\
&= 0 + \varepsilon^T JAS^{2n,2k} z + \varepsilon^T Jb + \frac{1}{2}\varepsilon^T JA\varepsilon \\
&= \varepsilon^T JS^{2n,2k} H_k^{2k,2k} z + \varepsilon^T Jb + \varepsilon^T J\zeta_{k+1} v_{k+1} e_{2k}^T z + \frac{1}{2}\varepsilon^T JA\varepsilon \\
&= \varepsilon^T JS^{2n,2k} H_k^{2k,2k} z + \varepsilon^T JS^{2n,2k} e_1 + H_3(t) \\
&= \varepsilon^T JS^{2n,2k} \dot{z} + H_3(t).
\end{aligned}
\tag{3.1}
$$

Next we want to show that $H_3(t) \equiv 0$. Based on the constructing of the symplectic Lancozs method, we have

$$
\begin{aligned}
S^{2n,2k^T} J^n S^{2n,2k} &= J^k \\
S^{2n,2n^T} J^n S^{2n,2k} &= \tilde{J}^{2n,2k},
\end{aligned}
\tag{3.2}
$$

where

$$
\tilde{J}^{2n,2k} = \begin{bmatrix} 0^{k,k} & I^{k,k} \\ 0^{n-k,k} & 0^{n-k,k} \\ -I^{k,k} & 0^{k,k} \\ 0^{n-k,k} & 0^{n-k,k} \end{bmatrix},
\tag{3.3}
$$

and

$$
\begin{aligned}
Z_i &= z_i, i = 1, 2, ..., k \\
Z_i &= z_i, i = n+1, 2, ..., n+k.
\end{aligned}
\tag{3.4}
$$

Thus,

$$
\begin{aligned}
\varepsilon^T JS^{2n,2k} &= (S^{2n,2n}\dot{Z} - S^{2n,2k} z)^T JS^{2n,2k} \\
&= \dot{Z}^T \tilde{J}^{2n,2k} - z^T J^k \\
&= [-Z_{n+1}, ..., -Z_{n+k}, Z_1, ..., Z_k] - z^T J^k \\
&= 0.
\end{aligned}
\tag{3.5}
$$

Equation (3.5) shows that the error term is J-orthognal to $S^{2n,2k}$. From equation (3.1) and (3.5) we get

$$H_3(t) \equiv 0. \tag{3.6}$$

The above results (3.6) shows that the non-autonomuns Hamiltonian system (2.2) is in fact a Hamiltonian system with a constant enenrgy.

4. Apply Trapezoidal rule and Midpoint rule to the error equation

Denote the constant matrix $\zeta_{k+1}v_{k+1}e_{2k}^T$ in the error equation (2.2) as B. Apply midpoint rule to the error equation (2.2), we get the iteration formular

$$\varepsilon_{n+1}^M = \varepsilon_n^M + \frac{hA}{2}(\varepsilon_n^M + \varepsilon_{n+1}^M) + hBz(\frac{t_n + t_{n+1}}{2}) \tag{4.1}$$

Apply trapezoidal rule to the error equation (2.2), we get the iteration formular

$$\varepsilon_{n+1}^T = \varepsilon_n^T + \frac{hA}{2}(\varepsilon_n^T + \varepsilon_{n+1}^T) + hB\frac{z(t_n) + z(t_{n+1})}{2} \tag{4.2}$$

The exact solution for equation (1.7) is

$$z(t) = e^{H_k^{2k,2k}t}z_0, \tag{4.3}$$

where z_0 is the vector $H_k^{2k,2k^{-1}}J^{k^{-1}}S^{2n,2k^T}J^n b$. Apparently $z(t)$ is not linear about t. Thus, ε_{n+1}^T is different from ε_{n+1}^M, which shows that Trapezoidal rule and Midpoint rule will behaviour differently on the error equation (2.2). Similarly, Trapezoidal rule and Midpoint rule will behaviour differently on equation (2.4).

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.