AMATH 586 SPRING 2020
MIDTERM EXAM — DUE MAY 15 ON GITHUB BY 11PM

SHANNON DOW

Be sure to do a `git pull` to update your local version of the `amath-586-2020` repository.

This entire exam concerns system of ODEs called the *Toda lattice*. The system is defined using positions p_j, $j = 0, \pm 1, \pm 2, \ldots$ and momenta q_j, $j = 0, \pm 1, \pm 2, \ldots$:

$$\begin{aligned} q_j'(t) &= p_j(t), \\ p_j'(t) &= e^{-(q_j(t)-q_{j-1}(t))} - e^{-(q_{j+1}(t)-q_j(t))}, \quad j = 0, \pm 1, \pm 2, \ldots. \end{aligned} \tag{1}$$

This is, as defined, an infinite-dimensional ODE system. We will consider finite-dimensional approximations.

Problem 1: Define new variables

$$\begin{aligned} a_j(t) &= \frac{1}{2} e^{-(q_{j+1}(t)-q_j(t))/2}, \\ b_j(t) &= -\frac{1}{2} p_j(t), \quad j = 0, \pm 1, \pm 2, \ldots. \end{aligned} \tag{2}$$

Using (2), first show that the Toda lattice (1) can be written as

$$\begin{aligned} a_j'(t) &= a_j(t)(b_{j+1}(t) - b_j(t)), \\ b_j'(t) &= 2(a_j^2(t) - a_{j-1}^2(t)), \quad j = 0, \pm 1, \pm 2, \ldots. \end{aligned} \tag{3}$$

Now consider the time-dependent tridiagonal matrices:

$$T(t) = \begin{bmatrix} \ddots & \ddots & & & \\ \ddots & b_{j-1}(t) & a_{j-1}(t) & & \\ & a_{j-1}(t) & b_j(t) & a_j(t) & \\ & & a_j(t) & b_{j+1}(t) & \ddots \\ & & & \ddots & \ddots \end{bmatrix}, \; S(t) = \begin{bmatrix} \ddots & \ddots & & & \\ \ddots & 0 & a_{j-1}(t) & & \\ & -a_{j-1}(t) & 0 & a_j(t) & \\ & & -a_j(t) & 0 & \ddots \\ & & & \ddots & \ddots \end{bmatrix}$$

Now, show that (3) is equilvalent to

$$T'(t) = S(t)T(t) - T(t)S(t). \tag{4}$$

Hint: Fix j and consider

$$e_j^T S(t)T(t)e_k \text{ and } e_j^T T(t)S(t)e_k, \quad k = j-2, j-1, j, j+1, j+2,$$

where e_j denotes the standard basis vector that is all zero except for a one in the jth entry. Despite the fact that the matrices are bi-infinite, you only need to track the $(j-1)$th, jth and $(j+1)$th entries of vectors such as $e_j^T S(t)$ and $T(t)e_k$.

Solution:

First, take the derivatives of $a_j(t)$ and $b_j(t)$

$$a_j'(t) = \frac{1}{2}e^{-(q_{j+1}(t)-q_j(t))/2}(-\frac{1}{2}q_{j+1}'(t) + \frac{1}{2}q_j'(t))$$

$$b_j'(t) = -\frac{1}{2}p_j'(t) = -\frac{1}{2}e^{-(q_j(t)-q_{j-1}(t))} - e^{-(q_{j+1}(t)-q_j(t))}$$

Additional relationships:

$$q_j'(t) = p_j(t) = -2b_j(t)$$
$$a_j^2(t) = \frac{1}{4}e^{-(q_{j+1}(t)-q_j(t))}$$
$$a_{j-1}^2(t) = \frac{1}{4}e^{-(q_j(t)-q_{j-1}(t))}$$

Thus we can rewrite

$$p_j'(t) = e^{-(q_j(t)-q_{j-1}(t))} - e^{-(q_{j+1}(t)-q_j(t))}$$
$$-2b_j'(t) = 4a_{j-1}^2(t) - 4a_j^2(t)$$
$$\boxed{b_j'(t) = 2(a_j^2(t) - a_{j-1}^2(t))}$$

To get the first part of (1), we must solve the $a_j'(t)$ for $q_j'(t)$

$$a_j'(t) = \frac{1}{2}e^{-(q_{j+1}(t)-q_j(t))/2}(-\frac{1}{2}q_{j+1}'(t) + \frac{1}{2}q_j'(t))$$
$$a_j'(t) = \frac{1}{4}q_j'(t)e^{-(q_{j+1}(t)-q_j(t))/2} - \frac{1}{4}q_{j+1}'(t)e^{-(q_{j+1}(t)-q_j(t))/2}$$
$$\frac{1}{4}q_j'(t)e^{-(q_{j+1}(t)-q_j(t))/2} = a_j'(t) + \frac{1}{4}q_{j+1}'(t)e^{-(q_{j+1}(t)-q_j(t))/2}$$
$$q_j'(t) = 4a_j'(t)e^{(q_{j+1}(t)-q_j(t))/2} + q_{j+1}'(t)$$

We know from (1) that $q_j'(t) = p_j(t)$where $p_j(t) = -2b_j(t)$

$$4a_j'(t)e^{(q_{j+1}(t)-q_j(t))/2} + q_{j+1}'(t) = -2b_j(t)$$
$$4a_j'(t)e^{(q_{j+1}(t)-q_j(t))/2} = 2b_{j+1}(t) - 2b_j(t)$$
$$a_j'(t) = \frac{1}{2}e^{(q_{j+1}(t)-q_j(t))/2}(b_{j+1}(t) - b_j(t))$$
$$\boxed{a_j'(t) = a_j(t)(b_{j+1}(t) - b_j(t))}$$

$$ST = \begin{bmatrix} \ddots & \ddots & & & \\ \ddots & 0 & a_{j-1}(t) & & \\ & -a_{j-1}(t) & 0 & a_j(t) & \\ & & -a_j(t) & 0 & \ddots \\ & & & \ddots & \ddots \end{bmatrix} * \begin{bmatrix} \ddots & \ddots & & & \\ \ddots & b_{j-1}(t) & a_{j-1}(t) & 0 & \\ & a_{j-1}(t) & b_j(t) & a_j(t) & \\ & 0 & a_j(t) & b_{j+1}(t) & \ddots \\ & & & \ddots & \ddots \end{bmatrix}$$

$$
\begin{aligned}
ST_{j,j-1} &= -a_{j-1}(t)b_{j-1}(t) \\
ST_{j,j} &= -a_{j-1}^2(t) + a_j^2(t) \\
ST_{j,j+1} &= a_j(t)b_{j+1}(t)
\end{aligned}
$$

$$
TS = \begin{bmatrix}
\ddots & \ddots & & & \\
\ddots & b_{j-1}(t) & a_{j-1}(t) & 0 & \\
 & a_{j-1}(t) & b_j(t) & a_j(t) & \\
 & 0 & a_j(t) & b_{j+1}(t) & \ddots \\
 & & & \ddots & \ddots
\end{bmatrix} * \begin{bmatrix}
\ddots & \ddots & & & \\
\ddots & 0 & a_{j-1}(t) & 0 & \\
 & -a_{j-1}(t) & 0 & a_j(t) & \\
 & 0 & -a_j(t) & 0 & \ddots \\
 & & & \ddots & \ddots
\end{bmatrix}
$$

$$
\begin{aligned}
TS_{j,j-1} &= -b_j(t)a_{j-1}(t) \\
TS_{j,j} &= a_{j-1}^2(t) - a_j^2(t) \\
TS_{j,j+1} &= b_j(t)a_j(t)
\end{aligned}
$$

$$
\begin{aligned}
(ST - TS)_{j,j-1} &= -a_{j-1}(t)(b_j(t) - b_{j-1}(t)) = -a'_{j-1}(t) \\
(ST - TS)_{j,j} &= -2(a_{j-1}^2(t) + a_j^2(t)) = b'_j(t) \\
(ST - TS)_{j,j+1} &= a_j(t)(b_{j+1(t)} - b_j(t)) = a'_j(t)
\end{aligned}
$$

Since T' = ST - TS takes the form

$$
T'(t) = \begin{bmatrix}
\ddots & \ddots & & & \\
\ddots & b'_{j-1}(t) & a'_{j-1}(t) & & \\
 & a'_{j-1}(t) & b'_j(t) & a'_j(t) & \\
 & & a'_j(t) & b'_{j+1}(t) & \ddots \\
 & & & \ddots & \ddots
\end{bmatrix}
$$

Thus, the two are equivalent.

Problem 2: One finite-dimensional approximation of (4) is to just take a finite section (a square subblock on the diagonal) of both T, P:

$$T_N(t) = \begin{bmatrix} b_1(t) & a_1(t) & & & \\ a_1(t) & b_2(t) & a_2(t) & & \\ & a_2(t) & b_3(t) & \ddots & \\ & & \ddots & \ddots & a_{N-1}(t) \\ & & & a_{N-1}(t) & b_N(t) \end{bmatrix},$$

$$S_N(t) = \begin{bmatrix} 0 & a_1(t) & & & \\ -a_1(t) & 0 & a_2(t) & & \\ & -a_2(t) & 0 & \ddots & \\ & & \ddots & \ddots & a_{N-1}(t) \\ & & & -a_{N-1}(t) & 0. \end{bmatrix}$$

The finite section choice can be understood by formally setting $q_0 = -\infty$ and $q_{N+1} = +\infty$ and then performing the change of variables (2).

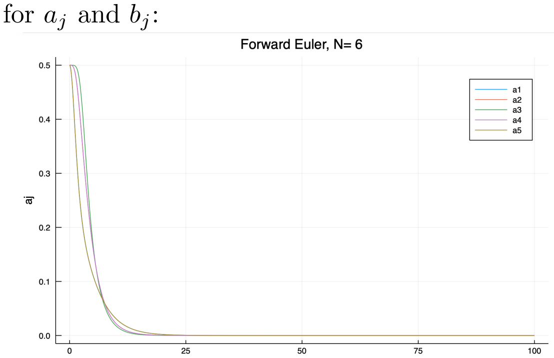
With initial conditions $b_j(0) = 0$, $a_j(0) = 1/2, j = 1, 2, \ldots, N$ and $N = 6$, use your favorite time-stepping method to solve

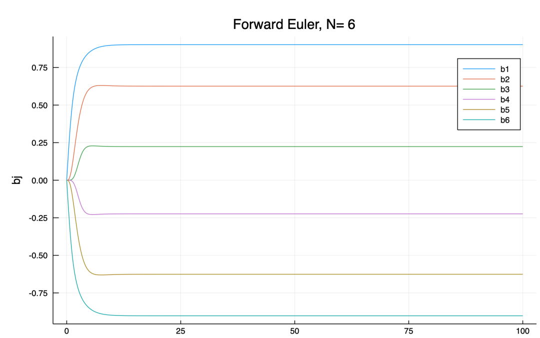
$$T_N'(t) = S_N(t)T_N(t) - T_N(t)S_N(t),$$

to $t = 100$ and plot the solution. You should notice something striking about the solution. You might want to look at eigenvalues of $T_N(0)$. Comment on this. Repeat this with $b_j(0) = -2$ and $a_j(0) = 1$, $j = 1, 2, \ldots, N$ and $N = 12$.

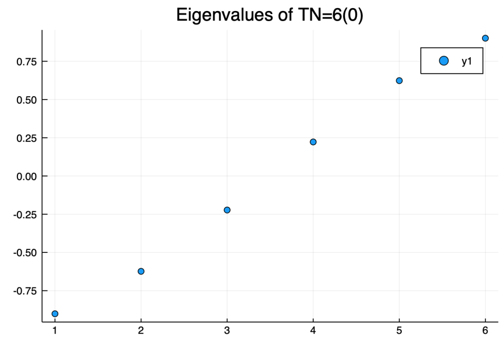
Solution

Using Forward Euler for N=6 and $a_j(0) = 1/2$ $b_j(0) = 0$ we get the following plots for a_j and b_j:

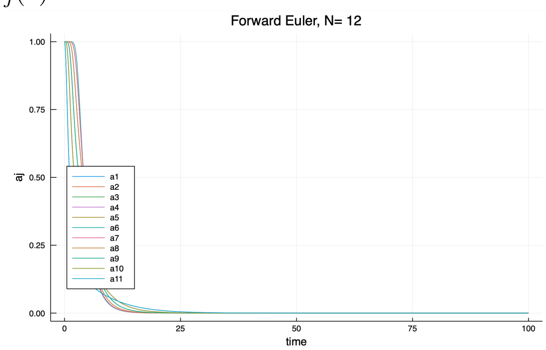


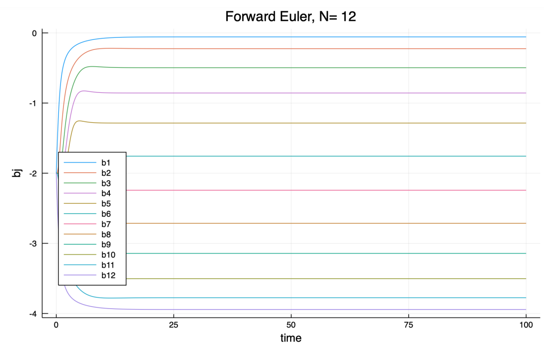


We can see that the b_j converge to the eigenvalues of $T_N(0)$

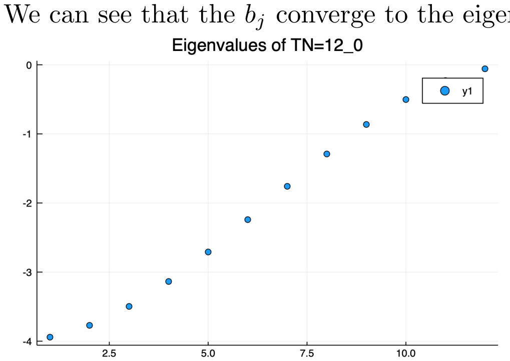


We can see this pattern again for N=12 with initial conditions $a_j(0) = 1$ and $b_j(0) = -2$





We can see that the b_j converge to the eigenvalues of $T_N(0)$



The code for this can be seen in the Jupyter Notebook. I additionally used Runge Kutta order 4 to verify the results. The b_j converge to the corresponding eigenvalues of TN(0). The a_j approach zero making T approach a tridiagonal matrix where the eigenvalues are the main diagonal.

Problem 3: The Toda lattice in the finite-section case is a Hamiltonian system with Hamiltonian

$$H(p, q) = \frac{1}{2}p_N^2 + \sum_{j=1}^{N-1} \left[\frac{1}{2}p_j^2 + e^{-(q_{j+1}-q_j)} \right].$$

This means that the equations of motion for $q_j(t)$ and $p_j(t)$ can also be written as

$$
\begin{aligned}
p_j'(t) &= -\frac{\partial H}{\partial q_j}(p(t), q(t)), \\
q_j'(t) &= \frac{\partial H}{\partial p_j}(p(t), q(t)),
\end{aligned} \tag{5}
$$

where $p(t) = (p_j(t))_{j=1}^N$ and $q(t) = (q_j(t))_{j=1}^N$. And, by the chain rule, H is conserved:

$$\frac{d}{dt}H(p(t), q(t)) = 0.$$

Sympletic numerical integrators for Hamiltonian systems are designed to preserve conserved quantities and geometric properties of systems they approximate. We can summarize the system (5) as

$$p'(t) = J(q(t)), \quad q'(t) = K(p(t)).$$

One symplectic method is the so-called Störmer–Verlet method and it is given by

$$
\begin{aligned}
P^* &= P^n + \frac{k}{2}J(Q^n), \\
Q^{n+1} &= Q^n + kK(P^*), \\
P^{n+1} &= P^* + \frac{k}{2}J(Q^{n+1}).
\end{aligned}
$$

Convert the initial data $b_j(0) = 0$ and $a_j(0) = 1/2$ for $j = 1, 2, \ldots, N$ to $q_j(0), p_j(0)$ for $j = 1, 2, \ldots, N$ and solve the system with the Störmer-Verlet method. Perform a convergence study at $t = 1$ for time steps $k = 2^{-j}$, $j = 1, 2, 3, 4, 5, 6$ (see `https://github.com/trogdoncourses/amath-586-2020/blob/master/notebooks/Astability.ipynb`) to determine the order of the method.

Some hints:

- Since the a_j,b_j variables depend only on a difference of the q_j. You can set one value, say $q_1(0)$, to be whatever value you wish.
- You also might want to write a function to convert between a_j, b_j and p_j, q_j. Here is a `Julia` implementation:

```
to_a = (p,q) -> .5*exp.(-(q[2:end]-q[1:end-1])/2)
to_b = (p,q) -> -.5*p
to_p = (a,b) -> -2*b
function to_q(a,b) # chooses q[1] = 0
    q = fill(0.,length(b))
    q[2:end] = -2*log.(2*a)
    cumsum(q)
end
```

- Here is a `Julia` implementation of J and K:

```
function J(q)
    out = fill(0.,length(q))
    temp = exp.(q[1:end-1] - q[2:end])
    out[1:end-1] -= temp
```

```
        out[2:end] += temp
        out
    end

    function K(p)
        p
    end
```

Just for your information: A second order method will satisfy:

$$\text{error at time } T \sim C_T k^2.$$

And the constant C_T is incredibly important as T increases. Symplectic methods can be used to keep C_T from growing too rapidly and they are very important in, say, planetary dynamics over long time scales.

Solution

```
Error reduction ratio b 5.004373667590925
Error reduction ratio a 4.210418508497765
Error reduction ratio b 4.214793382315254
Error reduction ratio a 4.086837471396729
Error reduction ratio b 4.106216033838947
Error reduction ratio a 4.153618518510122
Error reduction ratio b 4.274062623228083
```

Based on this, we can conclude that the method is second order accurate.

Problem 4: (Extra credit) Form a finite-dimensional approximation of (1) using the boundary condition $q_0(t) = q_{N+1}(t)$ and performing the change of variables (2). Update the matrices T_N and S_N for the periodic case.