Symplectic integration methods

Marc R. Roussel

November 17, 2019

Euler's method

- Suppose that we have a differential equation

$$\frac{d\mathbf{z}}{dt} = \mathbf{f}(\mathbf{z}).$$

- If the equation does not have an analytic solution, we might want to integrate it numerically, as we have been doing with XPPAUT.
- The simplest possible method is Euler's method.
- There are two parts to Euler's method:
  1. Approximate the derivative by

$$\frac{d\mathbf{z}}{dt} \approx \frac{\mathbf{z}(t+\Delta t) - \mathbf{z}(t)}{\Delta t}$$

  2. Assume that the right-hand side is approximately constant over the interval $[t, t+\Delta t]$, and equal to $\mathbf{f}(\mathbf{z}(t))$.

Euler's method (continued)

- Notation: In the simplest case, we would take steps of fixed size $\Delta t = h$.
  Denote $x(t + jh)$ by x_j.
- Euler's method is therefore

$$\frac{\mathbf{z}_{j+1} - \mathbf{z}_j}{h} = \mathbf{f}(\mathbf{z}_j)$$

  or

$$\mathbf{z}_{j+1} = \mathbf{z}_j + h\mathbf{f}(\mathbf{z}_j)$$

- This is an explicit method: If I know $\mathbf{z}_j$, I can directly calculate $\mathbf{z}_{j+1}$ by just evaluating the above formula.

Euler's method applied to a Hamiltonian system

- The harmonic oscillator has Hamiltonian

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

- The resulting rate equations are

$$\begin{aligned}\frac{dx}{dt} &= \frac{\partial H}{\partial p} = \frac{p}{m} \\ \frac{dp}{dt} &= -\frac{\partial H}{\partial x} = -kx\end{aligned}$$

- Euler's method applied to these equations gives

$$\begin{aligned}x_{j+1} &= x_j + hp_j/m \\ p_{j+1} &= p_j - hkx_j\end{aligned}$$

Euler's method and the value of the Hamiltonian

- The exact dynamics conserves the value of the Hamiltonian. Does Euler's method?
- Consider

$$\begin{aligned} H(x_{j+1}, p_{j+1}) &= \frac{1}{2}kx_{j+1}^2 + \frac{p_{j+1}^2}{2m} \\ &= \frac{k}{2}\left(x_j + hp_j/m\right)^2 + \frac{1}{2m}\left(p_j - hkx_j\right)^2 \\ &= \frac{1}{2}kx_j^2 + \frac{p_j^2}{2m} + \frac{k}{m}h^2\left(\frac{1}{2}kx_j^2 + \frac{p_j^2}{2m}\right) \\ &= H(x_j, p_j)\left(1 + \frac{k}{m}h^2\right). \end{aligned}$$

- The value of the Hamiltonian therefore grows by a factor of $1 + h^2k/m$ at each step.
  Not good.

A chained Euler's method

- In the standard Euler's method, we update the equations in parallel.
- What if we "chained" the evaluations as follows?

$$x_{j+1} = x_j + hp_j/m$$
$$p_{j+1} = p_j - hkx_{j+1}$$

- This method is called the semi-implicit Euler method (although it's actually an explicit method).
- If you substitute (x_{j+1}, p_{j+1}) into the Hamiltonian, you will find that this method does not preserve the Hamiltonian.

A chained Euler's method (continued)

- However, consider the perturbed Hamiltonian

$$H_p = \frac{1}{2}kx^2 + \frac{p^2}{2m} + \frac{hk}{2m}xp$$

$$\begin{aligned}
H_p(x_{j+1}, p_{j+1}) &= \frac{1}{2}kx_{j+1}^2 + \frac{p_{j+1}^2}{2m} + \frac{hk}{2m}x_{j+1}p_{j+1} \\
&= \frac{1}{2}kx_{j+1}^2 + \frac{1}{2m}\left(p_j - hkx_{j+1}\right)^2 + \frac{hk}{2m}x_{j+1}\left(p_j - hkx_{j+1}\right) \\
&= \frac{1}{2}kx_{j+1}^2 + \frac{p_j^2}{2m} - \frac{hk}{2m}x_{j+1}p_j \\
&= \frac{1}{2}k\left(x_j + hp_j/m\right)^2 + \frac{p_j^2}{2m} - \frac{hk}{2m}p_j\left(x_j + hp_j/m\right) \\
&= \frac{1}{2}kx_j^2 + \frac{p_j^2}{2m} + \frac{hk}{2m}x_jp_j
\end{aligned}$$

A chained Euler's method (continued)

- Thus
$$H_p = \frac{1}{2}kx^2 + \frac{p^2}{2m} + \frac{hk}{2m}xp$$
is a conserved quantity of this numerical scheme.
- Because of this conserved quantity, the numerical solutions don't display a consistently growing energy.
- Moreover, the perturbation to the true Hamiltonian depends on h, so H_p becomes closer to H as we decrease h.
- Such a numerical scheme is called symplectic.
In fact, this numerical method is often called the symplectic Euler method.

Hamiltonian-preserving methods

- We can do better and design methods that preserve the exact Hamiltonian.
- To do this, we have to return to Hamilton's equations of motion.
- We have (for a system with one degree of freedom)

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}$$

- We approximate both sides of this equation by finite differences:

$$\begin{aligned}\frac{dx}{dt} &\approx \frac{x_{j+1} - x_j}{h} \\ \frac{\partial H}{\partial p} &\approx \frac{H(x_j, p_{j+1}) - H(x_j, p_j)}{p_{j+1} - p_j}\end{aligned}$$

Hamiltonian-preserving methods (continued)

- Setting the two derivatives equal to each other, we get the equation

$$\frac{x_{j+1} - x_j}{h} = \frac{H(x_j, p_{j+1}) - H(x_j, p_j)}{p_{j+1} - p_j}$$

- Note that we don't know p_{j+1}.
- Applying similar reasoning to dp/dt, we get

$$\frac{p_{j+1} - p_j}{h} = -\frac{H(x_{j+1}, p_{j+1}) - H(x_j, p_{j+1})}{x_{j+1} - x_j}$$

  (Note the use of p_{j+1} in the right-hand side, analogous to the semi-implicit Euler method.)
- These equations involve the Hamiltonian evaluated at the unknown $j+1$ point.
- We call numerical schemes such as this implicit schemes because, in general, we can't write a simple formula for (x_{j+1}, p_{j+1}).

Hamiltonian-preserving methods (continued)

- The first of the two equations of the numerical scheme can be rearranged to

$$\frac{1}{h}(x_{j+1}-x_j)(p_{j+1}-p_j)=H(x_j,p_{j+1})-H(x_j,p_j)$$

- Similarly, the second equation gives

$$\frac{1}{h}(x_{j+1}-x_j)(p_{j+1}-p_j)=H(x_j,p_{j+1})-H(x_{j+1},p_{j+1})$$

- Therefore

$$H(x_{j+1},p_{j+1})=H(x_j,p_j)$$

- So we can exactly preserve the value of the Hamiltonian at the cost of using an implicit method.

Summary: numerical schemes for Hamiltonian systems

- So we have two good schemes for Hamiltonian systems, and one bad one.
- Bad: explicit Euler method
- Better: symplectic semi-implicit Euler method

$$x_{j+1} = x_j + h \left.\frac{\partial H}{\partial p}\right|_{(x_j, p_j)}$$

$$p_{j+1} = p_j - h \left.\frac{\partial H}{\partial x}\right|_{(x_{j+1}, p_j)}$$

- Even better: Hamiltonian-preserving implicit method

$$\frac{x_{j+1} - x_j}{h} = \frac{H(x_j, p_{j+1}) - H(x_j, p_j)}{p_{j+1} - p_j}$$

$$\frac{p_{j+1} - p_j}{h} = -\frac{H(x_{j+1}, p_{j+1}) - H(x_j, p_{j+1})}{x_{j+1} - x_j}$$