Simulation Methods

Numerical Methods for Ordinary Differential Equations

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The leap-frog scheme I

We want to integrate the differential equation $\ddot{q} = f(q)$ or

$$\begin{aligned} \dot{p} &= f(q), \\ \dot{q} &= p \end{aligned}$$

Replacing the second derivative by the central second-order difference quocient:

$$q_{n+1} - 2q_n + q_{n-1} = h^2 f(q_n).$$

It is called the **Störmer method**, the **leap-frog method** or the **Verlet method**. We can approximate the derivative $p = \dot{q}$ by

$$p_n = \frac{q_{n+1} - q_{n-1}}{2h}, \quad \text{and} \quad p_{n+1/2} = \frac{q_{n+1} - q_n}{h},$$

and we obtain the one-step method:

The leap-frog scheme II

One step leap-frog method

$$\begin{aligned} p_{n+1/2} &= p_n + \frac{h}{2} f(q_n), \\ q_{n+1} &= q_n + h p_{n+1/2}, \\ p_{n+1} &= p_{n+1/2} + \frac{h}{2} f(q_{n+1}) \end{aligned} \tag{1}$$

From the definitions, we obtain

$$\begin{aligned} p_{n+1/2} - p_{n-1/2} &= hf(q_n), \\ p_{n+1/2} + p_{n-1/2} &= 2p_n \end{aligned} \tag{2}$$

$$\begin{aligned} p_{n+3/2} - p_{n+1/2} &= hf(q_{n+1}), \\ p_{n+3/2} + p_{n+1/2} &= 2p_{n+1} \end{aligned} \tag{3}$$

- We get first equation of (1) by elimination of $p_{n-1/2}$ in (2).
- For the second equation of (1), we use the definition of $p_{n+1/2}$.
- Using (3) and eliminating $p_{n+3/2}$ we obtain the third equation of (1).

The leap-frog scheme III

Comment

If one is not interested in the values p_n of the derivative, the first and the third equation can be replaced by

$$p_{n+1/2} = p_{n-1/2} + hf(q_n).$$

The Kepler problem and the leap-frog method I

We want to compute the motion of two bodies which attract each other.

- We choose one of the bodies at the origin.
- As the motion stays in a plane, we use coordinates $q = (q_1, q_2)$ for the position of the second body.

Newton's law yields:

$$\ddot{q}_1 = -\frac{q_1}{(q_1^2 + q_2^2)^{3/2}}, \qquad \ddot{q}_2 = -\frac{q_2}{(q_1^2 + q_2^2)^{3/2}}.$$

Equivalent to a Hamiltonian system with the Hamiltonian

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}, \qquad p_i = \dot{q}_i.$$

The Kepler problem and the leap-frog method II

Comment

A 2d-dimensional Hamiltonian system has the form

$$\dot{p}_k = -\frac{\partial H}{\partial q_k}(p, q), \qquad \dot{q}_k = \frac{\partial H}{\partial p_k}(p, q), \quad k = 1, \dots, d.$$

In general H is a first integral of the system, that is $H(p(t), q(t))$ is constant for any trajectory $(p(t), q(t))$.

The system has two first integrals:

- $H(p, q)$ (**energy**) and,
- $L(p, q) = q_1 p_2 - q_2 p_1$ (**angular momentum**).

Fact

The leap-frog method preserves both first integrals.

Leap-frog method for partitioned systems I

Consider a **partitioned system**:

$$
\begin{aligned}
\dot{u} &= a(u, v), \\
\dot{v} &= b(u, v)
\end{aligned}
$$

We will define the leap-frog method of a composition of two **partitioned Euler** or **symplectic Euler** methods:

$$
\begin{aligned}
u_{n+1} &= u_n + ha(u_n, v_{n+1}), \\
v_{n+1} &= v_n + hb(u_n, v_{n+1})
\end{aligned}
$$

and

$$
\begin{aligned}
u_{n+1} &= u_n + ha(u_{n+1}, v_n), \\
v_{n+1} &= v_n + hb(u_{n+1}, v_n)
\end{aligned}
$$

Leap-frog method for partitioned systems II

Comment

- *They are implicit Euler methods in one variable and explicit in the other.*
- *They have global order of convergence 1.*

Then we can compose these methods considering half step for both methods:

$$
\begin{aligned}
u_{n+1} &= u_{n+\frac{1}{2}} + \frac{h}{2} a(u_{n+\frac{1}{2}}, v_{n+1}) \\
v_{n+1} &= v_{n+\frac{1}{2}} + \frac{h}{2} b(u_{n+\frac{1}{2}}, v_{n+1})
\end{aligned}
$$

and

$$
\begin{aligned}
u_{n+\frac{1}{2}} &= u_n + \frac{h}{2} a(u_{n+\frac{1}{2}}, v_n) \\
v_{n+\frac{1}{2}} &= v_n + \frac{h}{2} b(u_{n+\frac{1}{2}}, v_n)
\end{aligned}
$$

Leap-frog method for partitioned systems III

We obtain the leap-frog method:

Leap-frog method 1

$$
\begin{aligned}
u_{n+\frac{1}{2}} &= u_n + \frac{h}{2} a(u_{n+\frac{1}{2}}, v_n) \\
v_{n+1} &= v_n + \frac{h}{2}\left(b(u_{n+\frac{1}{2}}, v_{n+1}) + b(u_{n+\frac{1}{2}}, v_n)\right) \\
u_{n+1} &= u_{n+\frac{1}{2}} + \frac{h}{2} a(u_{n+\frac{1}{2}}, v_{n+1})
\end{aligned}
$$

If we change the order of the composition

$$
\begin{aligned}
u_{n+1/2} &= u_n + \frac{h}{2} a(u_n, v_{n+1/2}) \\
v_{n+1/2} &= v_n + \frac{h}{2} b(u_n, v_{n+1/2})
\end{aligned}
$$

Leap-frog method for partitioned systems IV

and

$$
\begin{aligned}
u_{n+1} &= u_{n+1/2} + \frac{h}{2} a(u_{n+1}, v_{n+1/2}) \\
v_{n+1} &= v_{n+1/2} + \frac{h}{2} b(u_{n+1}, v_{n+1/2}),
\end{aligned}
$$

we obtain a second version of the leap-frog method:

Leap-frog method 2

$$
\begin{aligned}
v_{n+1/2} &= v_n + \frac{h}{2} b(u_n, v_{n+1/2}) \\
u_{n+1} &= u_n + \frac{h}{2} \left(a(u_n, v_{n+1/2}) + a(u_{n+1}, v_{n+1/2}) \right) \\
v_{n+1} &= v_{n+1/2} + \frac{h}{2} b(u_{n+1}, v_{n+1/2})
\end{aligned}
$$

Leap-frog method for partitioned systems V

Comment

Consider $\dot{x} = f(x)$, $x \in \mathbb{R}^n$, $f(x) \in \mathbb{R}^n$ *an* **autonomous system**.
Let $\Phi_t = \Phi_t(x)$ *be its* **flow**. *We know that*

$$\Phi_h(x) = \varphi(h; t, x), \ \textit{for any } t.$$

Then, the numerical integration method has to have the same property, that is

$$\tilde{\varphi}(h; t, x) = \tilde{\varphi}(h; 0, x), \quad \forall\, t.$$

Then, we can define

$$\tilde{\Phi}_h(x) = \tilde{\varphi}(h; 0, x).$$

Symplectic methods for Hamiltonian systems I

If we apply the previous methods to the differential equation

$$\begin{aligned} \dot{p} &= -H_q(p,q), \\ \dot{q} &= H_p(p,q) \end{aligned}$$

where $H_p = \nabla_p H$ and $H_q = \nabla_q H$, we obtain the partitioned Euler methods:

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \\ q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \end{aligned}$$

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{aligned}$$

and the leap-frog methods:

Symplectic methods for Hamiltonian systems II

$$
\begin{aligned}
p_{n+\frac{1}{2}} &= p_n - \frac{h}{2} H_q(p_{n+\frac{1}{2}}, q_n) \\
q_{n+1} &= q_n + \frac{h}{2}\left(H_p(p_{n+\frac{1}{2}}, q_{n+1}) + H_p(p_{n+\frac{1}{2}}, q_n)\right) \\
p_{n+1} &= p_{n+\frac{1}{2}} - \frac{h}{2} H_q(p_{n+\frac{1}{2}}, q_{n+1})
\end{aligned}
$$

$$
\begin{aligned}
q_{n+1/2} &= q_n + \frac{h}{2} H_p(p_n, q_{n+1/2}) \\
p_{n+1} &= p_n - \frac{h}{2}\left(H_q(p_n, q_{n+1/2}) + H_q(p_{n+1}, q_{n+1/2})\right) \\
q_{n+1} &= q_{n+1/2} + \frac{h}{2} H_p(p_{n+1}, q_{n+1/2})
\end{aligned}
$$

Symplectic methods for Hamiltonian systems III

Let us define the $2d \times 2d$ matrix

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix},$$

where I is the identity matrix of dimension d.

Definition

A linear map $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called **symplectic** *if $A^T JA = J$.*

Definition

A differentiable map $g : U \subset \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ (where U is an open set) is called symplectic if the Jacobian matrix $Dg(p, q)$ is everywhere symplectic, i.e., if

$$Dg(p, q)^T JDg(p, q) = J.$$

Symplectic methods for Hamiltonian systems IV

Theorem (Poincaré 1899)

Let $H(p,q)$ be a twice continously differentiable function on $U \subset \mathbb{R}^{2d}$. Then, for each fixed t, the flow φ_t is a symplectic transformation wherever it is defined.

Proof:

Note that we can write the Hamiltonian system as

$$\dot{y} = J^{-1}\nabla H(y),$$

where $\nabla H(y) = H'(y)^T$. The derivative $\partial\varphi_t/\partial y_0$ (with $y_0 = (p_0, q_0)$) is a solution of the variational equation

$$\dot{\Psi} = J^{-1}\nabla^2 H(\varphi_t(y_0))\Psi, \qquad \Psi(t_0) = I,$$

Symplectic methods for Hamiltonian systems V

where $\nabla^2 H(p,q)$ is the Hessian matrix of $H(p,q)$. Therefore, we obtain

$$\frac{d}{dt}\left(\left(\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{\partial\varphi_t}{\partial y_0}\right)\right) =$$

$$\left(\frac{d}{dt}\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{\partial\varphi_t}{\partial y_0}\right) + \left(\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{d}{dt}\frac{\partial\varphi_t}{\partial y_0}\right)$$

$$= \left(\frac{\partial\varphi_t}{\partial y_0}\right)^T \nabla^2 H(\varphi_t(y_0)) J^{-T} J\left(\frac{\partial\varphi_t}{\partial y_0}\right) +$$

$$\left(\frac{\partial\varphi_t}{\partial y_0}\right)^T \nabla^2 H(\varphi_t(y_0))\left(\frac{\partial\varphi_t}{\partial y_0}\right) = 0,$$

since $J^T = -J$ and $J^{-T}J = -I$. Then

$$\frac{\partial\varphi_t}{\partial y_0}(t_0) = I \;\Rightarrow\; \left(\frac{\partial\varphi_t}{\partial y_0}\right)^T J\left(\frac{\partial\varphi_t}{\partial y_0}\right) = J$$

Symplectic methods for Hamiltonian systems VI

Definition

A numerical one-step method is called symplectic if the one-step map $x_1 = \tilde{\Phi}_h(x_0)$ is symplectic whenever the method is applied to a smooth Hamilonian system.

Proposition

The symplectic Euler methods are symplectic.

Proof:

We consider only one case:

$$
\begin{aligned}
p_{n+1} &= p_n - hH_q(p_{n+1}, q_n), \\
q_{n+1} &= q_n + hH_p(p_{n+1}, q_n).
\end{aligned}
$$

Symplectic methods for Hamiltonian systems VII

Differentiation with respect to (p_n, q_n) yields

$$\left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right) = \begin{pmatrix} I & -hD_qH_q \\ 0 & I + hD_qH_p \end{pmatrix} + \begin{pmatrix} -hD_pH_q & 0 \\ hD_pH_p & 0 \end{pmatrix} \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right),$$

where $D_pH_p = H_{pp} = (H_{p_i,p_j})_{1\leq i,j\leq d}$, $D_qH_q = H_{qq} = (H_{q_i,q_j})_{1\leq i,j\leq d}$,

$$D_pH_q = H_{pq} = (H_{p_i,q_j})_{1\leq i,j\leq d}, \quad D_qH_p = H_{qp} = (H_{q_i,p_j})_{1\leq i,j\leq d} = H_{pq}^T,$$

and the matrices $H_{qp}, H_{pp}, \ldots$ are evaluated at (p_{n+1}, q_n). Then

$$\begin{pmatrix} I + hH_{pq} & 0 \\ -hH_{pp} & I \end{pmatrix} \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right) = \begin{pmatrix} I & -hH_{qq} \\ 0 & I + hH_{qp} \end{pmatrix},$$

This relation allows us to compute

$$\left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right) = \begin{pmatrix} (I + hH_{pq})^{-1} & -h(I + H_{pq})^{-1}H_{qq} \\ hH_{pp}(I + hH_{pq})^{-1} & -h^2H_{pp}(I + hH_{pq})^{-1}H_{qq} + I + hH_{qp} \end{pmatrix}$$

Symplectic methods for Hamiltonian systems VIII

and to check in a straightforward way the symplecticity condition

$$\left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right)^T J \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right) = J.$$

□

Comment

These methods are implicit for general Hamiltonian systems. For separable $H(p, q) = T(p) + U(q)$, *however, both variants turn out to be explicit.*

As the composition of symplectic maps is symplectic, and the leapfrog is a composition of two sympletic Euler methods we have

Theorem

The leapfrog (or Störmer-Verlet) schemes are symplectic of order of global convergence equal to 2.

Symplectic methods for Hamiltonian systems IX

Comment

The leap-frog methods are implicit for general Hamiltonian systems. For separable $H(p,q) = T(p) + U(q)$*, however, both variants turn out to be explicit.*

Definition

Consider a one-step numerical integration method for autonomous differential equations with map $\tilde{\Phi}_h(x) = \tilde{\Phi}(h,x)$. *The* **adjoint method** *is defined by the map* $\tilde{\Phi}_h^* = \tilde{\Phi}_{-h}^{-1}$. *We say that the method is* **symmetric** *if* $\tilde{\Phi}_h^* = \tilde{\Phi}_h$.

Comment

If Φ_h *is the flow of an autonomous ode then* $\Phi_{-h}^{-1} = \Phi_h$.

Symplectic methods for Hamiltonian systems X

Theorem

Let Φ_h be the exact flow of

$$\dot{x} = f(x), \qquad x(t_0) = x_0$$

and let $\tilde{\Phi}_h$ be a one-step method of order p satisfying

$$\tilde{\Phi}_h(x_0) = \Phi_h(x_0) + C(x_0)h^{p+1} + O(h^{p+2}).$$

The adjoint method $\tilde{\Phi}^*$ then has the same order and

$$\tilde{\Phi}_h^*(x_0) = \Phi_h(x_0) + (-1)^p C(x_0)h^{p+1} + O(h^{p+2}).$$

If the method is symmetric, its (maximal) order is even.

Symplectic methods for Hamiltonian systems XI

Proof.

We know that $\Phi_h(x) = x + O(h)$, and

$$\tilde{\Phi}_{-h}(\tilde{\Phi}^*_h(x)) - \tilde{\Phi}_{-h}(\Phi_h(x)) = x - \tilde{\Phi}_{-h}(\Phi_h(x)) =$$

$$(-1)^p C(\Phi_h(x))h^{p+1} + O(h^{p+2}) = (-1)^p C(x)h^{p+1} + O(h^{p+2}).$$

On the other hand,

$$\tilde{\Phi}_{-h}(\tilde{\Phi}^*_h(x)) - \tilde{\Phi}_{-h}(\Phi_h(x)) = F(h, \tilde{\Phi}^*_h(x), \Phi_h(x))(\tilde{\Phi}^*_h(x) - \Phi_h(x)) =$$

$$(I + O(h))(\tilde{\Phi}^*_h(x) - \Phi_h(x)),$$

which proves the first part of the theorem.
If $\tilde{\Phi}_h$ is symmetric then $(-1)^p C(x) = C(x)$, and, as $C(x) \neq 0$ we have that p is even.

$\square$

Symplectic methods for Hamiltonian systems XII

Proposition

The adjoint of the partitioned Euler method with function $\tilde{\Phi}_h$

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \\ q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \end{aligned}$$

is

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{aligned}$$

Symplectic methods for Hamiltonian systems XIII

Proof.

We have that

$$\begin{pmatrix} u_{n-1} \\ v_{n-1} \end{pmatrix} = \tilde{\Phi}_{-h}(u_n, v_n) = \begin{pmatrix} u_n - ha(u_n, v_{n-1}) \\ v_n - hb(u_n, v_{n-1}) \end{pmatrix},$$

and

$$\begin{pmatrix} u_n \\ v_n \end{pmatrix} = \tilde{\Phi}_{-h}^{-1}(u_{n-1}, v_{n-1}) = \begin{pmatrix} u_{n-1} + ha(u_n, v_{n-1}) \\ v_{n-1} + hb(u_n, v_{n-1}) \end{pmatrix}.$$

□

Comment

Let $\tilde{\Phi}_h$ be a symplectic Euler method. Then, the other one is its adjoint. Moreover the leapfrog methods are symmetric: $\tilde{\Phi}_{h/2} \circ \tilde{\Phi}^*_{h/2}$ and $\tilde{\Phi}^*_{h/2} \circ \tilde{\Phi}_{h/2}$, and of order two.

The Taylor method

Problem: find a function $x : [a, b] \to \mathbb{R}^m$ such that

$$\left\{ \begin{array}{rcl} x'(t) & = & f(t, x(t)), \\ x(a) & = & x_0, \end{array} \right.$$

Taylor method (one step method):

$$\begin{array}{rcl} x_0 & = & x(a), \\ x_{m+1} & = & x_m + x'(t_m)h + \cdots + \dfrac{x^{(p)}(t_m)}{p!} h^p, \end{array}$$

for $m = 0, \ldots, N-1$.

A first approach is to compute the derivatives by means of the direct application of the chain rule,

$$
\begin{aligned}
x'(t_m) &= f(t_m, x(t_m)), \\
x''(t_m) &= f_t(t_m, x(t_m)) + f_x(t_m, x(t_m))x'(t_m), \\
x'''(t_m) &= f_{tt}(t_m, x(t_m)) + 2f_{tx}(t_m, x(t_m))x'(t_m) \\
&\quad + f_{xx}(t_m, x(t_m))x'(t_m)^2 + f_x(t_m, x(t_m))x''(t_m)
\end{aligned}
$$

and so on.

These expressions have to be obtained explicitly for each equation we want to integrate.

Example

Van der Pol equation

$$\left.\begin{array}{rcl} x' & = & y, \\ y' & = & (1-x^2)y - x. \end{array}\right\}.$$

The nth order Taylor method for the initial value problem is

$$\begin{array}{rcl} x_{m+1} & = & x_m + x'_m h + \frac{1}{2!} x''_m h^2 + \cdots + \frac{1}{n!} x_m^{(n)} h^n, \\ y_{m+1} & = & y_m + y'_m h + \frac{1}{2!} y''_m h^2 + \cdots + \frac{1}{n!} y_m^{(n)} h^n. \end{array}$$

Here $x_m^{(i)} = x^{(i)}(t_m)$ and $y_m^{(i)} = y^{(i)}(t_m)$

There are several ways of obtaining the derivatives of the solution w.r.t. time.

Example

Van der Pol equation

$$\left.\begin{array}{rcl} x' &=& y, \\ y' &=& (1-x^2)y - x. \end{array}\right\}.$$

A standard way is to take derivatives on the differential equation,

$$\begin{array}{rcl} x'' &=& (1-x^2)y - x, \\ y'' &=& -2xy^2 + [(1-x^2)^2 - 1]y - x(1-x^2), \\ x''' &=& -2xy^2 + [(1-x^2)^2 - 1]y - x(1-x^2), \\ y''' &=& 2y^3 - 8x(1-x^2)y^2 + [4x^2 - 2 + (1-x^2)^3]y \\ && +x[1-(1-x^2)^2], \\ & \vdots & \end{array}$$

Note how the expressions become increasingly complicated.

These closed formulas allow for the evaluation of the derivatives at any point, so they have to be computed only once (for each vector field).

For a long time integration,

- the effort needed to produce these formulas is not relevant,
- the effort to *evaluate them is very relevant*

Automatic differentiation

There is an alternative procedure to compute derivatives:
Automatic differentiation

Automatic differentiation is a recursive algorithm to evaluate the derivatives of a closed expression on a given point.

Automatic differentiation does not produce closed formulas for the derivatives.

The standard reference book is:
A. Griewank: *Evaluating derivatives*, SIAM (2000).
ISBN: `0-89871-284-X`