Lecture 5: Geometrical numerical integration methods for differential equations

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Geometrical numerical integration for ODEs

- Geometric integration: numerical integration of a differential equation, while preserving one or more of its geometric properties exactly.
- Geometric properties of crucial importance in physical applications: preservation of energy, momentum, volume, symmetries, time-reversal symmetry, dissipation, and symplectic structure.
- Hamiltonian systems and methods that preserve their symplectic structure, invariants, symmetries, or volume.

Geometrical numerical integration for ODEs

- Structure preserving methods for Hamiltonian systems

  Hamiltonian systems: important class of differential equations with a geometric structure (symplectic flow);
- Preservation in the numerical discretization of the geometric structure $\rightarrow$ substantially better methods, especially when integrating over long times.
- In general, most geometric properties: not preserved by standard numerical methods.
- Motivations to preserve structure:
  - (i) Faster, simpler, more stable, and/or more accurate for some types of ODEs;
  - (ii) More robust and quantitatively better results than standard methods for the long-time integration of Hamiltonian systems.

Geometrical numerical integration for ODEs

- Symplectic methods: Consider the Hamiltonian system

$$\begin{cases} \dfrac{\mathrm{d}p}{\mathrm{d}t} = -\dfrac{\partial H}{\partial q}(p,q), \\ \dfrac{\mathrm{d}q}{\mathrm{d}t} = \dfrac{\partial H}{\partial p}(p,q), \\ p(0) = p_0, q(0) = q_0, \end{cases}$$

$p_0, q_0 \in \mathbb{R}^d$; Hamiltonian function $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$: $\mathcal{C}^1$ function.

Geometrical numerical integration for ODEs

- Hamiltonian systems:
  - DEFINITION:
    - Hamiltonian system with Hamiltonian H: first-order system of ODEs

$$\begin{cases} \dfrac{\mathrm{d}p}{\mathrm{d}t} = -\dfrac{\partial H}{\partial q}(p, q), \\ \dfrac{\mathrm{d}q}{\mathrm{d}t} = \dfrac{\partial H}{\partial p}(p, q). \end{cases}$$

  - EXAMPLE:
    - Harmonic oscillator with Hamiltonian

$$H(p, q) = \frac{1}{2}\frac{p^2}{m} + \frac{1}{2}kq^2;$$

      m and k: positive constants.
    - Given a potential V, Hamiltonian systems of the form:

$$H(p, q) = \frac{1}{2}p^\top M^{-1}p + V(q);$$

      M: symmetric positive definite matrix and $\top$: transpose.

Geometrical numerical integration for ODEs

- Equivalent expression for Hamiltonian systems:
  - $x = (p, q)^\top$ $(p, q \in \mathbb{R}^d)$;

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

    I: $d \times d$ identity matrix.
  - $J^{-1} = J^\top$.
  - Rewrite the Hamiltonian system in the form

$$\frac{\mathrm{d}x}{\mathrm{d}t} = J^{-1} \nabla H(x).$$

Geometrical numerical integration for ODEs

- Invariant for a system of ODEs:
  - DEFINITION:
    - $\Omega = I \times D$; $I \subset \mathbb{R}$ and $D \subset \mathbb{R}^{2d}$.
    - Consider
    $$\frac{\mathrm{d}x}{\mathrm{d}t} = f(t, x(t));$$
    - $f : \Omega \to \mathbb{R}^{2d}$.
    - $F : D \to \mathbb{R}$: invariant if $F(x(t)) = Constant$.
  - LEMMA:
    - Hamiltonian H: invariant of the associated Hamiltonian system.

Geometrical numerical integration for ODEs

- DEFINITION Symplectic linear mapping
  - Matrix $A \in \mathbb{R}^{2d} \times \mathbb{R}^{2d}$ (linear mapping from $\mathbb{R}^{2d}$ to $\mathbb{R}^{2d}$): symplectic if $A^\top J A = J$.
- DEFINITION Symplectic mapping
  - Differentiable map $g : U \to \mathbb{R}^{2d}$: symplectic if the **Jacobian matrix** $g'(p,q)$: everywhere symplectic, i.e., if

$$g'(p,q)^\top J g'(p,q) = J.$$

Geometrical numerical integration for ODEs

- THEOREM:
  - If g: symplectic mapping, then it preserves the Hamiltonian form of the equation.

Geometrical numerical integration for ODEs

- DEFINITION:
  - Flow:
$$\phi_t(p_0, q_0) = (p(t, p_0, q_0), q(t, p_0, q_0));$$
  - $\phi_t : U \to \mathbb{R}^{2d}$, $U \subset \mathbb{R}^{2d}$;
  - p_0 and q_0: initial data at $t = 0$.
- THEOREM: Poincaré's theorem
  - H: twice differentiable.
  - Flow ϕ_t: symplectic transformation.

Geometrical numerical integration for ODEs

- Symplecticity of the flow: characteristic property of the Hamiltonian system.
- THEOREM:
  - $f : U \to \mathbb{R}^{2d}$: continuously differentiable.
  - $\frac{\mathrm{d}x}{\mathrm{d}t} = f(x)$: locally Hamiltonian iff $\phi_t(x)$: symplectic for all $x \in U$ and for all sufficiently small t.

Geometrical numerical integration for ODEs

- DEFINITION:
  - Let $J := \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$.
  - Numerical one-step method

$$(p^{k+1}, q^{k+1}) = \Phi_{\Delta t}(p^k, q^k)$$

symplectic if the numerical flow $\Phi_{\Delta t}$: symplectic map:

$$\Phi'_{\Delta t}(p,q)^\top J \Phi'_{\Delta t}(p,q) = J,$$

for all (p,q) and all step sizes Δt.

Geometrical numerical integration for ODEs

- THEOREM:
  - Implicit Euler method:

$$\begin{cases} p^{k+1} = p^k - \Delta t \dfrac{\partial H}{\partial q}(p^{k+1}, q^k), \\ q^{k+1} = q^k + \Delta t \dfrac{\partial H}{\partial p}(p^{k+1}, q^k), \end{cases}$$

    symplectic.
  - Moreover, if $H(p, q) = T(p) + V(q)$ is separable, then the scheme: explicit.

Geometrical numerical integration for ODEs

- PROOF:
  - $\Phi_{\Delta t}$: numerical flow

$$\Phi'_{\Delta t}(p^k, q^k) = \frac{\partial(p^{k+1}, q^{k+1})}{\partial(p^k, q^k)}.$$

  - $\frac{\partial^2 H}{\partial p^2}$, $\frac{\partial^2 H}{\partial q^2}$, and $\frac{\partial^2 H}{\partial p^2}$ evaluated at (p^{k+1}, q^k):

$$\begin{pmatrix} I + \Delta t \dfrac{\partial^2 H}{\partial p \partial q} & 0 \\ -\Delta t \dfrac{\partial^2 H}{\partial p^2} & I \end{pmatrix} \Phi'_{\Delta t}(p^k, q^k) = \begin{pmatrix} I & -\Delta t \frac{\partial^2 H}{\partial q^2} \\ 0 & I + \Delta t \dfrac{\partial^2 H}{\partial p \partial q} \end{pmatrix}.$$

  - $\Rightarrow$ Symplecticity condition holds by computing $\Phi'_{\Delta t}(p^k, q^k)$.

Geometrical numerical integration for ODEs

- Variant of Euler scheme:

$$\begin{cases} p^{k+1} = p^k - \Delta t \dfrac{\partial H}{\partial q}(p^k, q^{k+1}), \\ q^{k+1} = q^k + \Delta t \dfrac{\partial H}{\partial p}(p^k, q^{k+1}). \end{cases}$$

- Symplectic and explicit for separable Hamiltonian functions.

Geometrical numerical integration for ODEs

- THEOREM:
  - Composition of two symplectic one-step methods: also symplectic.

Geometrical numerical integration for ODEs

- PROOF:
  - $\Phi_{\Delta t}^{(1)}$ and $\Phi_{\Delta t}^{(2)}$: numerical flows associated with two symplectic one-step methods.
  - $\Phi_{\Delta t} := \Phi_{\Delta t}^{(2)} \circ \Phi_{\Delta t}^{(1)}$.

Geometrical numerical integration for ODEs

- Compute: $x^* = \Phi^{(1)}_{\Delta t}(x)$,

$$
\begin{aligned}
(\Phi'_{\Delta t}(x))^\top J \Phi'_{\Delta t}(x) &= ((\Phi^{(2)}_{\Delta t})'(x^*)(\Phi^{(1)}_{\Delta t})'(x))^\top J (\Phi^{(2)}_{\Delta t})'(x^*)(\Phi^{(1)}_{\Delta t})'(x) \\
&= ((\Phi^{(1)}_{\Delta t})'(x))^\top ((\Phi^{(2)}_{\Delta t})'(x^*))^\top J (\Phi^{(2)}_{\Delta t})'(x^*)(\Phi^{(1)}_{\Delta t})'(x) \\
&= ((\Phi^{(1)}_{\Delta t})'(x))^\top J (\Phi^{(1)}_{\Delta t})'(x) = J.
\end{aligned}
$$

- $\Rightarrow$ Composition of symplectic one-step methods: symplectic one-step method.

Geometrical numerical integration for ODEs

- Leapfrog method (Verlet method and Strömer-Verlet method):

$$\begin{cases} p^{k+\frac{1}{2}} = p^k - \dfrac{\Delta t}{2} \dfrac{\partial H}{\partial q}(p^{k+\frac{1}{2}}, q^k), \\ q^{k+1} = q^k + \dfrac{\Delta t}{2} \left(\dfrac{\partial H}{\partial p}(p^{k+\frac{1}{2}}, q^k) + \dfrac{\partial H}{\partial p}(p^{k+\frac{1}{2}}, q^{k+1}) \right), \\ p^{k+1} = p^{k+\frac{1}{2}} - \dfrac{\Delta t}{2} \dfrac{\partial H}{\partial q}(p^{k+\frac{1}{2}}, q^{k+1}). \end{cases}$$

- THEOREM:
  - Leapfrog method: symplectic.

Geometrical numerical integration for ODEs

- PROOF:
  - Leapfrog method: composition of the symplectric Euler method

$$\left\{\begin{array}{lll} p^{k+\frac{1}{2}} & = & p^k - \dfrac{\Delta t}{2}\dfrac{\partial H}{\partial q}(p^{k+\frac{1}{2}}, q^k), \\ q^{k+\frac{1}{2}} & = & q^k + \dfrac{\Delta t}{2}\dfrac{\partial H}{\partial p}(p^{k+\frac{1}{2}}, q^k), \end{array}\right.$$

and its adjoint

$$\left\{\begin{array}{lll} q^{k+1} & = & q^{k+\frac{1}{2}} + \dfrac{\Delta t}{2}\dfrac{\partial H}{\partial p}(p^{k+\frac{1}{2}}, q^{k+1}), \\ p^{k+1} & = & p^{k+\frac{1}{2}} - \dfrac{\Delta t}{2}\dfrac{\partial H}{\partial q}(p^{k+\frac{1}{2}}, q^{k+1}). \end{array}\right.$$

  - Symplectic methods $\Rightarrow$ composition: also symplectic.

Geometrical numerical integration for ODEs

- DEFINITION:
  - Adjoint method $\Phi^*_{\Delta t}$ of a method $\Phi_{\Delta t}$: inverse map of the original method with reversed time step:

$$\Phi^*_{\Delta t} := \Phi^{-1}_{-\Delta t}.$$

- Replace Δt by $-\Delta t$ and exchange k and $k+1$.
- Properties:
  - $(\Phi^*_{\Delta t})^* = \Phi_{\Delta t}$;
  - $(\Phi^{(2)}_{\Delta t} \circ \Phi^{(1)}_{\Delta t})^* = (\Phi^{(1)}_{\Delta t})^* \circ (\Phi^{(2)}_{\Delta t})^*$;
  - $(\Phi_{\Delta t/2} \circ \Phi^*_{\Delta t/2})^* = \Phi_{\Delta t/2} \circ \Phi^*_{\Delta t/2}$.

Geometrical numerical integration for ODEs

- Preserving time-reversal symmetry and invariants
- Preserving time-reversal symmetry:
  - Leapfrog method: symmetric with respect to changing the direction of time;
  - Replacing Δt by $-\Delta t$ and exchanging the superscripts k and $k+1$ results in the same method.

Geometrical numerical integration for ODEs

- Symmetry property for the numerical one-step map $\Phi_{\Delta t} : (p^k, q^k) \mapsto (p^{k+1}, q^{k+1})$.
- DEFINITION:
  - Numerical one-step map $\Phi_{\Delta t}$: symmetric if

$$\Phi_{\Delta t} = \Phi^{-1}_{-\Delta t} (=: \Phi^*_{\Delta t}).$$

- Symmetry property: does not hold for the symplectic Euler methods.

Geometrical numerical integration for ODEs

- Implicit Euler method:

$$\left\{ \begin{array}{lcl} p^{k+1} & = & p^k - \Delta t \dfrac{\partial H}{\partial q}(p^{k+1}, q^k), \\ q^{k+1} & = & q^k + \Delta t \dfrac{\partial H}{\partial p}(p^{k+1}, q^k). \end{array} \right.$$

- Variant of Euler scheme:

$$\left\{ \begin{array}{lcl} p^{k+1} & = & p^k - \Delta t \dfrac{\partial H}{\partial q}(p^k, q^{k+1}), \\ q^{k+1} & = & q^k + \Delta t \dfrac{\partial H}{\partial p}(p^k, q^{k+1}). \end{array} \right.$$

Geometrical numerical integration for ODEs

- Time-symmetry of the leapfrog method $\Rightarrow$ important geometric property of the numerical map.
- $\Phi_{\Delta t}$: Symplectic Euler method;
- Leapfrog method: composed method:

$$\Phi_{\Delta t/2} \circ \Phi^*_{\Delta t/2}.$$

Geometrical numerical integration for ODEs

- Assume that

$$H(-p, q) = H(p, q).$$

- $H(p, q) = \frac{1}{2} p^\top M^{-1} p + V(q)$.
- $\Rightarrow$ Hamiltonian system: has the property that inverting the direction of the initial p_0 does not change the solution trajectory.
- Flow ϕ_t satisfies:

$$\phi_t(p_0, q_0) = (p, q) \Rightarrow \phi_t(-p, q) = (-p_0, q_0).$$

- $\Rightarrow \phi_t$: reversible with respect to the reflection $(p, q) \mapsto (-p, q)$.

Geometrical numerical integration for ODEs

- DEFINITION:
  - Numerical one-step map $\Phi_{\Delta t}$: reversible if

$$\Phi_{\Delta t}(p, q) = (\hat{p}, \hat{q}) \Rightarrow \Phi_{\Delta t}(-\hat{p}, \hat{q}) = (-p, q),$$

for all p, q and all Δt.

Geometrical numerical integration for ODEs

- Symmetry of the leapfrog method $\Leftrightarrow$ reversibility:

$$\Phi_{\Delta t}(p,q) = (\hat{p},\hat{q}) \Rightarrow \Phi_{-\Delta t}(-p,q) = (-\hat{p},\hat{q}).$$

- THEOREM:
  - If H satisfies: $H(-p,q) = H(p,q)$, then Leapfrog method: both symmetric and reversible.

Geometrical numerical integration for ODEs

- Preserving invariants
- DEFINITION:
  - Numerical one-step method: preserve the invariant F if $F(\Phi_{\Delta t}(p,q)) = \text{Constant}$ for all p, q and all Δt.
  - If $F = H$, then scheme preserves energy.
- THEOREM:
  - Leapfrog method: preserves linear invariants and quadratic invariants of the form

$$F(p,q) = p^\top (Bq + b).$$

Geometrical numerical integration for ODEs

- PROOF:
  - Linear invariant $F(p,q) = b^\top q + c^\top p$ s.t.

$$b^\top \frac{\partial H}{\partial p}(p,q) - c^\top \frac{\partial H}{\partial q}(p,q) = 0,$$

    for all p, q.
  - Multiplying the formulas for $\Phi_{\Delta t}(p,q)$ by $(c,b)^\top \Rightarrow$ conservation of linear invariants.

Geometrical numerical integration for ODEs

- Conservation of quadratic invariants of the form $F(p,q) = p^\top (Bq + b)$ $\Leftarrow$ Leapfrog method: composition of the two symplectic Euler methods.
- For the first half-step,

$$(p^{k+\frac{1}{2}})^\top (Bq^{k+\frac{1}{2}} + b) = (p^k)^\top (Bq^k + b).$$

- For the second half-step,

$$(p^{k+1})^\top (Bq^{k+1} + b) = (p^{k+\frac{1}{2}})^\top (Bq^{k+\frac{1}{2}} + b).$$

Geometrical numerical integration for ODEs

- In general: energy not preserved by the leapfrog method.
- Consider $H(p,q) = \frac{1}{2}(p^2 + q^2)$.
- $$\begin{pmatrix} p^{k+1} \\ q^{k+1} \end{pmatrix} = \begin{bmatrix} 1 - \frac{(\Delta t)^2}{2} & -\Delta t(1 - \frac{(\Delta t)^2}{4}) \\ \Delta t & 1 - \frac{(\Delta t)^2}{2} \end{bmatrix} \begin{pmatrix} p^{k} \\ q^{k} \end{pmatrix}.$$
- Propagation matrix: not orthogonal $\Rightarrow H(p,q)$: not preserved along numerical solutions.

Geometrical numerical integration for ODEs

- Consider the Hamiltonian

$$H(p,q) := \frac{1}{2}p^\top M^{-1}p + V(q),$$

M: symmetric positive definite matrix and the potential V: smooth function.

- Leapfrog method reduces to the explicit method

$$\begin{cases} p^{k+\frac{1}{2}} = p^k - \dfrac{\Delta t}{2}\nabla V(q^k), \\ q^{k+1} = q^k + \Delta t M^{-1} p^{k+\frac{1}{2}}, \\ p^{k+1} = p^{k+\frac{1}{2}} - \dfrac{\Delta t}{2}\nabla V(q^{k+1}). \end{cases}$$

Geometrical numerical integration for ODEs

- Hamiltonian: invariant under $p \mapsto -p$ and the corresponding Hamiltonian system: invariant under the transformation

$$\begin{bmatrix} p \\ t \end{bmatrix} \mapsto \begin{bmatrix} -p \\ -t \end{bmatrix}.$$

- Time-reversal symmetry: preserved by leapfrog method.

Geometrical numerical integration for ODEs

- Preserving volume
- Equality of mixed partial derivatives $\Rightarrow f := J^{-1}\nabla H$: divergence-free

$$\nabla \cdot f := \sum_{i=1}^{2d} \frac{\partial f_i}{\partial x_i} = 0.$$

- Associated flows of divergence-free vector fields: volume preserving.
- Given a map $\phi : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ and a domain Ω, by change of variables

$$\mathrm{vol}(\phi(\Omega)) = \int_\Omega |\det \phi'(y)|\, dy,$$

ϕ': Jacobian of ϕ.

- ϕ preserves volume provided that

$$|\det \phi'(y)| = 1 \quad \text{for } y \in \Omega.$$

Geometrical numerical integration for ODEs

- THEOREM: (Liouville's theorem)
  - Vector field f: divergence-free.
  - Flow ϕ_t: volume preserving map (for all t).

Geometrical numerical integration for ODEs

- Flow ϕ_t satisfies
$$\frac{d\phi_t(y)}{dt} = f(\phi_t(y)).$$
- Jacobian ϕ' satisfies
$$\frac{d\phi_t'(y)}{dt} = f'(\phi_t(y))\phi_t'(y).$$
- Assume ϕ_t': invertible $\Rightarrow$
$$\mathrm{t}r\left[\frac{d\phi_t'(y)}{dt}\phi_t'(y)^{-1}\right] = \mathrm{t}rf'(\phi_t(y)).$$

Geometrical numerical integration for ODEs

- Combining $\mathrm{tr} f' = \nabla \cdot f = 0$ and Jacobi's formula for the derivative of a determinant $\Rightarrow$

$$\mathrm{tr}\left[\frac{d\phi_t'(y)}{dt}\phi_t'(y)^{-1}\right] = \frac{1}{\det \phi_t'(y)}\frac{d}{dt}\det \phi_t'(y) = 0.$$

- $$\det \phi_t'(y) = \det \phi_{t=0}'(y) = 1.$$

Geometrical numerical integration for ODEs

- Jacobi's formula:

$$\frac{d}{dt}\det A(t) = \det A(t)\, \mathrm{t}r\big(A(t)^{-1}\frac{dA}{dt}(t)\big).$$

- Application:

$$\det e^{tB} = e^{t \mathrm{tr} B}.$$

Geometrical numerical integration for ODEs

- DEFINITION:
    - Numerical one-step method: volume preserving if $|\det \Phi'_{\Delta t}(p, q)| = 1$ for all p, q.
- Hamiltonian system: any symplectic numerical method preserves the volume.
- No standard methods can be volume-preserving for all divergence-free vector fields.

Geometrical numerical integration for ODEs

- EXAMPLE:
  - Consider the divergence-free problem

$$\begin{cases} \dfrac{dx}{dt} = Ax, \\ x(0) = x_0 \in \mathbb{R}^{2d}, \end{cases}$$

  $A \in \mathbb{M}_{2d}(\mathbb{R})$ and $\mathrm{tr} A = 0$.
  - Explicit and implicit Euler's schemes:

$$x^{k+1} = x^k + \Delta t A x^k,$$

$$x^{k+1} = x^k + \Delta t A x^{k+1},$$

  volume-preserving if and only if

$$|\det(I + \Delta t A)| = 1,$$

  and

$$|\det(I - \Delta t A)| = 1,$$

  respectively.

Geometrical numerical integration for ODEs

- Composition methods
- Hamilton system: divergence-free $\Rightarrow$

$$
\begin{aligned}
f_{2d}(x) &= f_{2d}(\overline{x}) + \int_{\overline{x}}^{x_{2d}} \frac{\partial f_{2d}}{\partial x_{2d}}\, dx_{2d} \\
&= f_{2d}(\overline{x}) - \int_{\overline{x}}^{x_{2d}} \left(\sum_{i=1}^{2d-1} \frac{\partial f_i(x)}{\partial x_i} \right) dx_{2d},
\end{aligned}
$$

$\overline{x}$: arbitrary point which can be chosen conveniently (e.g., if possible s.t. $f_{2d}(\overline{x}) = 0$).

Geometrical numerical integration for ODEs

- $\Rightarrow$

$$
\begin{aligned}
\frac{dx_1}{dt} &= f_1(x), \\
&\vdots \\
\frac{dx_{2d-1}}{dt} &= f_{2d-1}(x), \\
\frac{dx_{2d}}{dt} &= f_{2d}(\overline{x}) - \sum_{i=1}^{2d-1} \int_{\overline{x}}^{x_{2d}} \frac{\partial f_i(x)}{\partial x_i} \, dx_{2d}.
\end{aligned}
$$

Geometrical numerical integration for ODEs

- Splitting as the sum of $2d-1$ vector fields

$$\begin{aligned}
\frac{dx_i}{dt} &= 0, \quad i \neq j, 2d-1,\\
\frac{dx_j}{dt} &= f_j(x),\\
\frac{dx_{2d}}{dt} &= f_{2d}(\overline{x})\delta_{j,2d-1} - \int_{\overline{x}}^{x_{2d}} \frac{\partial f_j(x)}{\partial x_j}\, dx_{2d},
\end{aligned}$$

for $j = 1, \ldots, 2d-1$. Here δ: Kronecker delta function.

- Each of the $2d-1$ vector fields: divergence-free.

Geometrical numerical integration for ODEs

- Each of problem: corresponds to a two-dimensional Hamiltonian system

$$\begin{aligned} \frac{dx_j}{dt} &= \frac{\partial H_j}{\partial x_{2d}}, \\ \frac{dx_{2d}}{dt} &= -\frac{\partial H_j}{\partial x_j}, \end{aligned}$$

  with Hamiltonian

$$H_j(x) := f_{2d}(\overline{x})\delta_{j,2d-1}x_j - \int_{\overline{x}}^{x_{2d}} f_j(x)\, dx_{2d},$$

  treating x_i for $i \neq j, 2d$ as fixed parameters.
- Each of the two-dimensional problems: can either be solved exactly (if possible), or approximated with a symplectic integrator $\Phi_{\Delta t}^{(j)}$.
- Volume-preserving integrator for f:

$$\Phi_{\Delta t} = \Phi_{\Delta t}^{(1)} \circ \Phi_{\Delta t}^{(2)} \circ \ldots \circ \Phi_{\Delta t}^{(2d-1)}.$$

Geometrical numerical integration for ODEs

- Splitting methods
- Consider a Hamiltonian system:

$$\frac{dx}{dt} = J^{-1}\nabla H(x), \quad H(x) = H_1(x) + H_2(x).$$

- Suppose the flows

$$\frac{dx}{dt} = J^{-1}\nabla H_1(x) \quad \text{and} \quad \frac{dx}{dt} = J^{-1}\nabla H_2(x),$$

  can be exactly integrated.
- Define the corresponding flow maps $\phi_t^{(1)}$ and $\phi_t^{(2)}$.

Geometrical numerical integration for ODEs

- Exact solution of a Hamiltonian system defines a symplectic map $\Rightarrow$

$$((\phi_t^{(1)})')^\top J(\phi_t^{(1)})' = J \quad \text{and} \quad ((\phi_t^{(2)})')^\top J(\phi_t^{(2)})' = J.$$

- Numerical method defined by composing the two exact flows:

$$\Phi_{\Delta t}(x) := \phi_{\Delta t}^{(2)} \circ \phi_{\Delta t}^{(1)}(x).$$

- Symplectic map: $x^* = \phi_{\Delta t}^{(1)}(x)$,

$$\begin{aligned}
(\Phi'_{\Delta t}(x))^\top J \Phi'_{\Delta t}(x) &= ((\phi_{\Delta t}^{(2)})'(x^*)(\phi_{\Delta t}^{(1)})'(x))^\top J(\phi_{\Delta t}^{(2)})'(x^*)(\phi_{\Delta t}^{(1)})'(x) \\
&= ((\phi_{\Delta t}^{(1)})'(x))^\top ((\phi_{\Delta t}^{(2)})'(x^*))^\top J(\phi_{\Delta t}^{(2)})'(x^*)(\phi_{\Delta t}^{(1)})'(x) \\
&= ((\phi_{\Delta t}^{(1)})'(x))^\top J(\phi_{\Delta t}^{(1)})'(x) = J.
\end{aligned}$$

- Composition of symplectic maps: again a symplectic map.

Geometrical numerical integration for ODEs

- EXAMPLE:
  - Consider the separable Hamiltonian $H(p, q) = T(p) + V(q)$.
  - Splitting the Hamiltonian H into T and $V \Rightarrow$
  - symplectic Euler method

$$\begin{cases} p^{k+1} = p^k - \Delta t \nabla V(q^k), \\ q^{k+1} = q^k + \Delta t \nabla T(p^{k+1}); \end{cases}$$

Geometrical numerical integration for ODEs

- Leapfrog method

$$\begin{cases} p^{k+\frac{1}{2}} = p^k - \dfrac{\Delta t}{2} \nabla V(q^k), \\ q^{k+1} = q^k + \Delta t \nabla T(p^{k+\frac{1}{2}}), \\ p^{k+1} = p^{k+\frac{1}{2}} - \dfrac{\Delta t}{2} \nabla V(q^{k+1}). \end{cases}$$

Geometrical numerical integration for ODEs

- Runge-Kutta methods:

$$(*)\begin{cases} x_{i,k} = x^k + (\Delta t)\sum_{j=1}^{m} a_{ij} f(x_{j,k}), \\ \\ x^{k+1} = x^k + (\Delta t)\sum_{i=1}^{m} b_i f(x_{i,k}). \end{cases}$$

- THEOREM:

  (i) All the Runge-Kutta methods preserve linear invariants;
  (ii) The Runge-Kutta method whose coefficients satisfy the condition

$$(**) \quad b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i, j = 1, \ldots m,$$

  preserves all quadratic invariants.

Geometrical numerical integration for ODEs

- PROOF:
    - Define $\Phi_{\Delta t}$ by $x^{k+1} = \Phi_{\Delta t}(x^k)$.
    - Let $F(x) = d^\top x$, $d \in \mathbb{R}^{2d}$.
    - Compute: $d^\top x$: invariant and hence $d^\top f(x_{i,k}) = 0 \Rightarrow$

$$F(\Phi_{\Delta t}(x^k)) = d^\top (x^k + \Delta t \sum_{i=1}^{m} b_i f(x_{i,k})) = d^\top x^k.$$

Geometrical numerical integration for ODEs

- Let $F(x) = x^\top C x$; C: symmetric $2d \times 2d$ matrix.
- F invariant $\Rightarrow x^\top C f(x) = 0 \quad$ for all x.
- Compute:

$$
\begin{aligned}
F(\Phi_{\Delta t}(x^k)) &= (x^k + \Delta t \sum_{j=1}^m b_j f(x_{j,k}))^\top C (x^k + \Delta t \sum_{i=1}^m b_i f(x_{i,k})) \\
&= (x^k)^\top C x^k + (\Delta t) \sum_{i=1}^m (x^k)^\top C b_i f(x_{i,k}) \\
&\quad + (\Delta t) \sum_{j=1}^m b_j f(x_{j,k})^\top C x^k \\
&\quad + (\Delta t)^2 \sum_{i,j=1}^m b_i b_j f(x_{j,k})^\top C f(x_{i,k}).
\end{aligned}
$$

Geometrical numerical integration for ODEs

- $(x_{i,k})^\top C f(x_{i,k}) = 0$, and

$$x^k = x^k + \Delta t \sum_{j=1}^m a_{ij} f(x_{j,k}) - \Delta t \sum_{j=1}^m a_{ij} f(x_{j,k}) = x_{i,k} - \Delta t \sum_{j=1}^m a_{ij} f(x_{j,k})$$

- $\Rightarrow$

$$F(\Phi_{\Delta t}(x^k)) = (x^k)^\top C x^k - (\Delta t)^2 \sum_{i,j=1}^m b_i a_{ij} f(x_{j,k})^\top C f(x_{i,k})$$

$$-(\Delta t)^2 \sum_{i,j=1}^m b_j a_{ji} f(x_{j,k})^\top C f(x_{i,k})$$

$$+(\Delta t)^2 \sum_{i,j=1}^m b_i b_j f(x_{j,k})^\top C f(x_{i,k})$$

$$= (x^k)^\top C x^k - (\Delta t)^2 \left(\sum_{i,j=1}^m (b_i a_{ij} + b_j a_{ji} - b_i b_j) f(x_{j,k})^\top C f(x_{i,k}) \right).$$

- $\Rightarrow$ Runge-Kutta method: preserves the quadratic invariant F provided that $(**)$ holds.

Geometrical numerical integration for ODEs

- H: invariant. If H is quadratic, then the energy is preserved by the Runge-Kutta method provided that condition $(**)$ holds.

Geometrical numerical integration for ODEs

- Characterization of symplectic Runge-Kutta methods:

  THEOREM:

  - Runge-Kutta method $(*)$ whose coefficients satisfy condition $(**)$: symplectic.

Geometrical numerical integration for ODEs

- PROOF:
  - Flow ϕ_t: symplectic transformation (if H: smooth enough).
  - Let $\Psi(t) := \frac{\partial \phi_t(x_0)}{\partial x_0} = \phi_t'$; x_0: initial condition.
  - $$(***)\begin{cases} \dfrac{d\Psi}{dt} = f'(x)\Psi, \\ \Psi(0) = I. \end{cases}$$
  - Apply a Runge-Kutta method to obtain the approximations x^{k+1} and Ψ^{k+1} from x^k and Ψ^k.

Geometrical numerical integration for ODEs

- $\Psi^\top J \Psi$: quadratic invariant $\Rightarrow$

$$(\Psi^k)^\top J \Psi^k = J \quad \text{for all } k.$$

- Suppose for a moment that

$$(****) \quad \Psi^{k+1} = \frac{\partial x^{k+1}}{\partial x^k}.$$

- $\Rightarrow$

$$\left(\frac{\partial x^{k+1}}{\partial x^k}\right)^\top J \frac{\partial x^{k+1}}{\partial x^k} = J,$$

- $\Rightarrow$ Runge-Kutta method whose coefficients satisfy condition $(**)$: symplectic.

Geometrical numerical integration for ODEs

- Proof of $(****)$:
  - Result of first applying $\Phi_{\Delta t}$ and then differentiating with respect to x^k: same as applying the same Runge-Kutta method to $(***)$.
  - Differentiation with respect to x^k $\Rightarrow$

$$\begin{cases} \dfrac{\partial x_{i,k}}{\partial x^k} = I + (\Delta t) \displaystyle\sum_{j=1}^{m} a_{ij} f'(x_{j,k}) \dfrac{\partial x_{j,k}}{\partial x^k}, \\ \dfrac{\partial x^{k+1}}{\partial x^k} = I + (\Delta t) \displaystyle\sum_{i=1}^{m} b_i f'(x_{i,k}) \dfrac{\partial x_{i,k}}{\partial x^k}. \end{cases}$$

Geometrical numerical integration for ODEs

- Multiplying the first equation in $(*)$ by $f'(x_{i,k}) \Rightarrow$ linear system in the unknowns $f'(x_{i,k})\frac{\partial x_{i,k}}{\partial x^k}$:

$$f'(x_{i,k})\frac{\partial x_{i,k}}{\partial x^k} = f'(x_{i,k})\Big(I + (\Delta t)\sum_{j=1}^{m} a_{ij} f'(x_{j,k})\frac{\partial x_{j,k}}{\partial x^k}\Big),$$

$$\frac{\partial x^{k+1}}{\partial x^k} = I + (\Delta t)\sum_{i=1}^{m} b_i f'(x_{i,k})\frac{\partial x_{i,k}}{\partial x^k}.$$

Geometrical numerical integration for ODEs

- Applying the same Runge-Kutta method to $(***)\Rightarrow$

$$\Psi_{i,k} = f'(x^k + \Delta t\sum_{j=1}^m a_{ij}x_{j,k})\Big(I + (\Delta t)\sum_{j=1}^m a_{ij}\Psi_{j,k}\Big),$$

$$\Psi^{k+1} = I + (\Delta t)\sum_{i=1}^m b_i\Psi_{i,k}.$$

- Same system but in the unknowns $\Psi_{i,k}, i = 1, \ldots, m$.
- Uniqueness of a solution for sufficiently small $\Delta t \Rightarrow$

$$\Psi_{i,k} = f'(x_{i,k})\frac{\partial x_{i,k}}{\partial x^k} \quad \text{for } i = 1, \ldots, m,$$

- $\Rightarrow (****)$.

Geometrical numerical integration for ODEs

- For arbitrary Hamiltonians: only known symplectic one-step numerical methods are the symplectic Runge-Kutta methods of the form

$$\begin{cases} x_{i,k} = x^k + (\Delta t) \sum_{j=1}^{m} a_{ij} f(t_{j,k}, x_{j,k}), \\ x^{k+1} = x^k + (\Delta t) \sum_{i=1}^{m} b_i f(t_{i,k}, x_{i,k}). \end{cases}$$

that satisfy the symplectic condition:

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i, j = 1, \ldots m.$$

Geometrical numerical integration for ODEs

- EXAMPLE:
  - Midpoint scheme:

$$x^{k+1} = x^k + \Delta t f\left(\frac{x^k + x^{k+1}}{2}\right),$$

symplectic, time-reversible, and preserves linear and quadratic invariants.

Geometrical numerical integration for ODEs

- Long-time behaviour of numerical solutions
- Energy: not exactly preserved by the leapfrog method.
- Approximately preserved.
- Symplecticity of a one-step numerical method $\Rightarrow$ approximate conservation of energy over very long times for general Hamiltonian systems.

Geometrical numerical integration for ODEs

- THEOREM:
  - For an analytic Hamiltonian H and a symplectic one-step numerical method $\Phi_{\Delta t}$ of order n, if the numerical trajectory remains in a compact subset, then there exist $h > 0$ and $\Delta t^* > 0$ s.t., for $\Delta t \leq \Delta t^*$,

$$H(p^k, q^k) = H(p^0, q^0) + O((\Delta t)^n),$$

  for exponentially long times $k\Delta t \leq e^{\frac{h}{\Delta t}}$. Here, $(p^{k+1}, q^{k+1}) = \Phi_{\Delta t}(p^k, q^k)$.

- Proof via backward error analysis.
- Idea: deduce the long-time behavior estimate from properties of the solution of the equation corresponding to an approximation $H_{\Delta t}$ of H.