Geometric Numerical Integration: Hamiltonian Systems, Symplectic Transformations

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Overview

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- Symplectic Transforms
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- Geometric Interpretation of Symplecticity for non linear mappings
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- main result: Poincaré’s Theorem
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- Geometric Interpretation of Symplecticity for non linear mappings
- main result: Poincaré’s Theorem
- Preservation of Hamiltonian character under symplectic transformations
Suppose, that the position of a mechanical system with $d$ degrees of freedom described by

$$q = (q_1, \ldots, q_d)^T,$$

as generalized coordinates, such as cartesian coordinates, angles etc. We suppose, that the kinetic energy is of the form

$$T = T(q, \dot{q})$$

and the potential energy is of the form

$$U = U(q).$$

We then define $L = T - U$ as the corresponding Lagrangian of the system.
The coordinates $q_1(t), \ldots, q_d(t)$, then obey the set of differential equations

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}_k} \right) - \frac{\partial L}{\partial q_k} = 0, \quad \text{for } k = 1, \ldots, d.$$ 

Numerical or analytical integration of this system therefore allows one to predict the motion of the system, given the initial values.
Examples

Newton’s second law

Let $m$ be a mass point in $\mathbb{R}^3$ with Cartesian coordinates $(x_1, x_2, x_2)^T$. We have $T = \frac{1}{2}m(\dot{x}_1^2 + \dot{x}_2^2 + \dot{x}_3^2)$. Suppose, the point moves in a conservative force field $F(x) = -\nabla U(x)$. Calculation of the Lagrangian equations leads to $m\ddot{x} - F(x) = 0$, which is Newton’s second law.
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Newton’s second law

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Pendulum

Take $\alpha$ as the generalized coordinate. Since $x = l \sin(\alpha)$ and $y = -l \cos(\alpha)$, we find for the kinetic energy $T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) = \frac{1}{2}ml^2\dot{\alpha}^2$ and for the potential energy $U = mgy = -mgl \cos(\alpha)$. The Lagrangian equations then lead to $ml^2\ddot{\alpha} + \frac{g}{l} \sin(\alpha) = 0$, the pendulum equation.
Hamilton’s Canonical Equations

Hamilton simplified the structure of Lagrange’s equations. He introduced the **conjugate momenta**:

\[ p_k = \frac{\partial L}{\partial \dot{q}_k} \quad \text{for } k = 1, \ldots, d \]  

and defined the Hamiltonian as

\[ H(p, q) := p^T \dot{q} - L(q, \dot{q}), \]

by expressing every \( \dot{q} \) as a function of \( p \) and \( q \), i.e. \( \dot{q} = \dot{q}(p, q) \). Here it is, required that (1) defines, for every \( q \), a continuously differentiable bijection: \( \dot{q} \leftrightarrow p \). This map is called **Legendre Transformation**.
Equivalence of Hamilton’s and Lagrange’s equations

Theorem

Lagrange’s equations are equivalent to Hamilton’s equations

\[ \dot{p}_k = -\frac{\partial H}{\partial q_k}(p, q) \]
\[ \dot{q}_k = \frac{\partial H}{\partial p_k}(p, q), \]

for \( k = 1, \ldots, d \).
Case of quadratic $T$

Assume $T = \frac{1}{2} \dot{q}^T M(q) \dot{q}$ quadratic, where $M(q)$ is a symmetric and positive definite matrix. For a fixed $q$ we have $p = M(q) \dot{q}$. Replacing $\dot{q}$ by $M^{-1}(q)p$ in the definition of the Hamiltonian leads to

$$H(p, q) = p^T M^{-1}(q)p - L(q, M^{-1}(q))$$

$$= p^T M^{-1}(q)p - \frac{1}{2} p^T M^{-1}(q)p + U(q)$$

$$= \frac{1}{2} p^T M^{-1}(q)p + U(q),$$

which is the total energy of the system. For quadratic kinetic energies, the Hamiltonian therefore represents the total energy.
A first property of Hamiltonian systems is, that the Hamiltonian is a first integral for Hamilton’s equations. Another very important property, which will be shown later, is the symplecticity of its flow. The basic objects we study are two-dimensional parallelograms in $\mathbb{R}^{2d}$. Suppose, that a parallelogram is spanned by two vectors

$$
\xi = \begin{pmatrix} \xi^p \\ \xi^q \end{pmatrix}, \quad \eta = \begin{pmatrix} \eta^p \\ \eta^q \end{pmatrix} \quad \xi^p, \xi^q, \eta^p, \eta^q \in \mathbb{R}^d,
$$

in the $p, q$-space. Therefore, the parallelogram is defined as

$$
P := \{ t\xi + s\eta \mid 0 \leq t \leq 1, 0 \leq s \leq 1 \}$$
For $d = 1$ consider the oriented area
or. $\text{area}(P) := \det \begin{pmatrix} \xi^p & \eta^p \\ \xi^q & \eta^q \end{pmatrix} = \xi^p \xi^q - \eta^p \eta^q$. For $d > 1$ replace it by the sum of the oriented areas of the projections of $P$ onto the coordinate planes $(p_i, q_i), i = 1, \ldots, d$:

$$\omega(\xi, \eta) := \sum_{i=1}^d \det \begin{pmatrix} \xi^p & \eta^p \\ \xi^q & \eta^q \end{pmatrix} = \sum_{i=1}^d (\xi^p \xi^q - \eta^p \eta^q).$$

This defines a bilinear map acting on vectors in $\mathbb{R}^{2d}$. It will play a central role for Hamiltonian systems. In matrix notation:

$$\omega(\xi, \eta) = \xi^T J \eta \quad \text{where} \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$
A linear mapping $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called \textit{symplectic} if

$$A^T J A = J \iff \omega(A\xi, A\eta) = \omega(\xi, \eta) \forall \xi, \eta \in \mathbb{R}^{2d}.$$
Symplecticity

Definition

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In the case of $d = 1$, where $\omega(\xi, \eta)$ represents the area of $P$, symplecticity of a linear mapping $A$ is therefore the area preservation of $A$. 
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Differentiable functions can locally be approximated by linear mappings, therefore the following definition is reasonable.
Symplecticity

**Definition**

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

\[
g'(p, q)^T J g'(p, q) = J
\]

or

\[
\omega(g'(p, q)\xi, g'(p, q)\eta) = \omega(\xi, \eta) \quad \forall \, \xi, \eta \in \mathbb{R}^{2d}.
\]
Consider a 2-dimensional sub-manifold \( M \) of the 2\( d \)-dimensional set \( U \). Suppose, that \( M = \psi(K) \), where \( K \subseteq \mathbb{R}^2 \) is a compact set and let \( \psi(s, t) \) be a continuously differentiable function. The sub-manifold \( M \) can then be considered as the limit of a union of small parallelograms, each spanned by the vectors

\[
\frac{\partial \psi}{\partial s}(s, t) \, ds \quad \text{and} \quad \frac{\partial \psi}{\partial t}(s, t) \, dt.
\]

We take for each parallelogram the sum over the oriented areas of its projections onto the \((p_i, q_i)\) plane. Then we sum over all parallelograms. In the limit we get the following:

\[
\Omega(M) = \iint_K \omega \left( \frac{\partial \psi}{\partial s}(s, t), \frac{\partial \psi}{\partial t}(s, t) \right) \, ds \, dt.
\]
Lemma

*If the mapping $g : U \rightarrow \mathbb{R}^{2d}$ is symplectic on $U$ then it preserves the expression $\Omega(M)$.***
Geometric Interpretation of Symplecticity for non linear mappings

Lemma

*If the mapping $g : U \rightarrow \mathbb{R}^{2d}$ is symplectic on $U$ then it preserves the expression $\Omega(M)$."

Notation

With the Lemma we’re now ready to prove the main result of my speech. Notation:

$$y = (p, q)$$
$$\dot{y} = J^{-1} \nabla H(y) = J^{-1} H'(y)^T$$

For the flow of the Hamiltonian system: $\varphi_t : U \rightarrow \mathbb{R}^{2d}$, we have the mapping, that advances the solution in time.
Poincaré’s Theorem

Theorem (Poincaré, 1899)

Let $H(p, q)$ be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. Then, for each fixed $t$, the flow $\varphi_t$ is a symplectic transformation wherever it is defined.
A differential equation $\dot{y} = f(y)$ is called *locally Hamiltonian* if $\forall \, y_0 \in U \, \exists \text{ a neighborhood where } f(y) = J^{-1} \nabla H(y)$, for a function $H$. The symplecticity of the flow is a characteristic property of Hamiltonian systems.
Characteristic property of Hamiltonian systems

**locally Hamiltonian**

Symplecticity of the flow is characteristic property of Hamiltonian systems. A diff eq $\dot{y} = f(y)$ is called **locally Hamiltonian** if $\forall \ y_0 \in U \ \exists$ a neighborhood where $f(y) = J^{-1} \nabla H(y)$, for a function $H$.

**Theorem**

Let $f : U \rightarrow \mathbb{R}^{2d}$ be continuously differentiable. Then the following is equivalent:

- $\dot{y} = f(y)$, it’s flow $\varphi_t(y)$
- is locally Hamiltonian $\iff$ is symplectic $\forall \ y \in U$, $t$ sufficiently small.
Integrability Lemma

**Lemma**

Let $D \subset \mathbb{R}^n$ be open and $f : D \rightarrow \mathbb{R}^n$ be continuously differentiable. Assume that the Jacobian $f'(y)$ is symmetric for all $y \in D$. Then for every $y_0 \in D$ there exists a neighborhood and a function $H(y)$ such that

$$f(y) = \nabla H(y)$$

on this neighborhood.
Hamiltonian systems under coordinate changes

**Theorem**

Let \( \psi : U \rightarrow V \) be a change of coordinates such that \( \psi \) and \( \psi^{-1} \) are continuously differentiable. If \( \psi \) is symplectic, the Hamiltonian system \( \dot{y} = J^{-1}\nabla H(y) \) becomes in the new variables \( z = \psi(y) \):

\[
\dot{z} = J^{-1}\nabla K(z) \quad \text{where} \quad K(z) = H(y). \quad (\star)
\]

Conversely, if \( \psi \) transforms every Hamiltonian system to another Hamiltonian system via \((\star)\), then \( \psi \) is symplectic.