# Geometric Numerical Integration:

## Hamiltonian Systems, Symplectic Transformations

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# Overview

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- Geometric Interpretation of Symplecticity for non linear mappings

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- Geometric Interpretation of Symplecticity for non linear mappings
- main result: Poincaré's Theorem

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- Symplectic Transforms
- Geometric Interpretation of Symplecticity for non linear mappings
- main result: Poincaré's Theorem
- Preservation of Hamiltonian character under symplectic transformations

# introduction

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.

# introduction



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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## 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:

$$p_k = \frac{\partial L}{\partial \dot{q}_k} \quad \text{for } k = 1, \dots, d \tag{1}$$

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

$$
\begin{aligned}
H(p,q) =& p^T M^{-1}(q)p - L(q, M^{-1}(q)) \\
&= p^T M^{-1}(q)p - \frac{1}{2}p^T M^{-1}(q)p + U(q) \\
&= \frac{1}{2}p^T M^{-1}(q)p + U(q),
\end{aligned}
$$

which is the total energy of the system. For quadratic kinetic energies, the Hamiltonian therefore represents the total energy.

# introduction





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

$$P := \{t\xi + s\eta \mid 0 \leq t \leq 1, 0 \leq s \leq 1\}$$

# introduction

For $d = 1$ consider the oriented area

or. 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 $(p_i, q_i)$, $i = 1, \dots, d$:

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

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

$$\omega(\xi, \eta) = \xi^T J \eta \quad \text{where } J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} .$$

# Symplecticity

## Definition

A linear mapping $A : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called symplectic if

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

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Differentiable functions can locally be approximated by linear mappings, therefore the following definition is reasonable.

# Symplecticitiy



## Definition

A differentiable map $g : U \to \mathbb{R}^{2d}$, 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

$$\omega(g'(p,q)\xi, g'(p,q)\eta) = \omega(\xi,\eta) \ \forall\ \xi,\eta \in \mathbb{R}^{2d}\,.$$

# Geometric Interpretation of Symplecticity for non linear mappings



Consider a 2-dimensional sub-manifold $M$ of the $2d$-dimensional set $U$. Suppose, that $M = \psi(K)$, where $K \subset \mathbb{R}^2$ 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:

$$\Omega(M) = \iint_K \omega\left(\frac{\partial \psi}{\partial s}(s,t), \frac{\partial \psi}{\partial t}(s,t)\right) dsdt.$$

# Geometric Interpretation of Symplecticity for non linear mappings



**Lemma**

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

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## Notation

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

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

For the flow of the Hamiltonian system: $\varphi_t : U \to \mathbb{R}^{2d}$, 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.*

# 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 $H$.

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## Theorem

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

$$\begin{array}{rcl} \dot{y} = f(y) & & \text{it's flow } \varphi_t(y) \\ \text{is locally Hamiltonian} & \Leftrightarrow & \text{is symplectic } \forall\ y \in U, \\ & & t \text{ sufficiently small.} \end{array}$$

# Integrability Lemma



**Lemma**

*Let $D \subset \mathbb{R}^n$ be open and $f : D \to \mathbb{R}^n$ 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 $\psi : U \to V$ 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 $z = \psi(y)$:*

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

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