Geometric numerical integration.

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I Introduction.

As already studied at the beginning of the course, there is a substantial difference between dissipative and conservative dynamical systems. This difference in structure results in a different strategy as far as numerical methods are concerned. For example, we have observed that solving for the Arenstorf orbit using even advanced Runge-Kutta methods such as DOPRI5 with time adaptation and error control is fine as long as we aim at solving for a solution on a relatively short time scale. When it comes to solving for several periods another strategy has to be found. The purpose of the present course inspired from the monograph of HAIRER LUBICH and WANNER (Springer, 2006) and its emanation: the course taught by E. HAIRER at TU München during the Winter 2009-2010 (See the documents on the website). The first part is dedicated to the proper definition of conservative dynamical system: Hamiltonian systems, symplectic transformation, that is area preserving; then, having in mind the key properties at the continuous level, we focus on the design of numerical methods, which are supposed to reproduce such properties.

II Hamiltonian Systems.

We focus on Hamiltonian systems. Given p, q in $\mathbb{R}^d$ and $H(p,q)$ a sufficiently smooth function of $(p,q) \in \mathbb{R}^d \times \mathbb{R}^d$ called the Hamiltonian or "total energy", the dynamics of the system given by $(p(t), q(t))$ satisfies:

$$\begin{cases} d_t p = -\partial_q H(p,q) \\ d_t q = +\partial_p H(p,q) \end{cases} \qquad (1)$$

II.1. Derivation from Lagrangian dynamics.

At the beginning of the course, we had introduce the Lagrangian of the dynamics and the motion of the system was governed by Lagrange's equations. Actually, when a mechanical system has its position described by d degrees of freedom $(q_1 - q_d)^t \in \mathbb{R}^d$ called generalized coordinates (coordinates, angles, ---), the Lagrangian of the system is given by

$$(2) \quad \begin{cases} \mathcal{L} = T - U, & T = T(q, d_t q) \text{ kinetic energy.} \\ \mathcal{L} = \mathcal{L}(q, d_t q), & U = U(q) \text{ potential energy.} \end{cases}$$

Lagrange's equation reads:

$$(3) \quad d_t\left(\partial_{d_t q} \mathcal{L}\right) = \partial_q \mathcal{L}$$

which are the Euler-Lagrange equations of the variational problem

$$S = \int_a^b \mathcal{L}(q(t), d_t q(t))\, dt$$

Hamilton (see Historical papers) simplified the structure of Lagrange's equations, leading to a formulation with a very symmetrical role of variables:

- by introducing conjugate momenta (Poisson's variables)

$$(4) \quad p_k = \partial_{d_t q} \mathcal{L}(q, d_t q) \qquad k = 1, \ldots, d$$

- considering the Hamiltonian:

$$(5) \qquad H := p^t d_t q - \mathcal{L}(q, d_t q).$$

where $\mathcal{L}$ was a functional of $(q, d_t q)$, H is a functional of p and q obtained by expressing $d_t q$ as a function of q and p using (4)

Let us underline that it is required here that (4) defines for every q a continuously differentiable bijection $d_t q \leftrightarrow p$, which is called the Legendre transform.

THEOREME. Lagrange's equations (3) are equivalent to Hamilton's equations.

$$(6) \begin{cases} d_t p_k = -\partial_{q_k} H(p, q) \\ d_t q_k = \partial_{p_k} H(p, q) \end{cases} \qquad k = 1, \ldots, d.$$

Proof: From (5), we have

$$\partial_p H = d_t q^t + p^t \partial_p (d_t q) - \partial_{d_t q} \mathcal{L} \, \partial_p (d_t q)$$

$$\partial_q H = p^t \partial_q (d_t q) - \partial_q \mathcal{L} - \partial_{d_t q} \mathcal{L} \, \partial_q (d_t q)$$

Since $\partial_{d_t q} \mathcal{L}^t = p$, $\partial_p H = (d_t q)^t$ and $\partial_q H = -\partial_q \mathcal{L}$ $\square$

When the kinetic energy is a quadratic function of $d_t q$, that is

$$T(q, d_t q) = \frac{1}{2} d_t q^t \, \Gamma(q) \, d_t q$$

where $\Gamma(q)$ is a symmetric and positive definite matrix, we have
$p(q, d_t q) = \Gamma(q) \, d_t q$ so that $d_t q(q, p) = \Gamma(q)^{-1} p$

Thus, the Hamiltonian is given by.

$$H(p,q) = p^t \Gamma(q)^{-1} p - \mathcal{L}(q, \Gamma(q)^{-1} p).$$

$$H(p,q) = \frac{1}{2} p^t \Gamma(q)^{-1} p + U(q). \tag{7}$$

and the Hamiltonian reads $H = U + T$, which is the total energy.

II.2 Energy conservation and first integrals - Examples.

Definition: A non constant function $I(y)$ is a first integral of the dynamical system $d_t y = f(y)$ if.

$$I'(y) \, f(y) = 0$$

This is equivalent to the property that every solution $y(t)$ of $d_t y = f(y)$ satisfies $I(y) = $ Constant.

Proposition: Conservation of the total energy: For Hamiltonian systems, the Hamiltonian $H(p,q)$ is a first integral.

Some mechanical systems admit other invariants or first integrals.
For example, a system of N particles interacting pairwise with potential forces depending on the distance of the particles, is a Hamiltonian system with

$$(8) \quad \mathcal{H}(p,q) = \frac{1}{2}\sum_{i=1}^{N} \frac{1}{m_i} p_i^t p_i + \sum_{i=2}^{N}\sum_{j=1}^{i-1} V_{ij}(\|q_i - q_j\|)$$

where $(p_i, q_i) \in \mathbb{R}^3 \times \mathbb{R}^3$ represent the momentum and position of the particles i of mass m_i and V_{ij} $i>j$ is the interaction potential between ith and jth particle. The equations of motion read:

$$(9) \quad \begin{cases} d_t q_i = \frac{1}{m_i} p_i \\ d_t p_i = \sum_{j=1}^{N} \nu_{ij}(q_i - q_j) \end{cases}$$

where for $i>j$ we have $\nu_{ij} = \nu_{ji} = -V'_{ij}(r_{ij})/r_{ij}$
$r_{ij} = \|q_i - q_j\|$.

For such a dynamical system, verify that the linear momentum of the system

$$P = \sum_{i=1}^{N} p_i$$

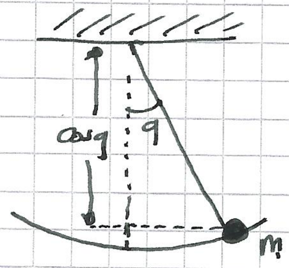
as well as the angular momentum

$$L = \sum_{i=1}^{N} q_i \wedge p_i$$

are conserved quantities since $\nu_{ij} = \nu_{ji}$, that is by symmetry.

Let us also briefly come back to the case of the pendulum, we have studied using Lagrangian dynamics at the beginning of the course.
The mathematical pendulum (mass $m=1$, massless rod of length $l=1$ with a gravitational acceleration of $g=1$) is a system with one degree of freedom with Hamiltonian

$$H(p,q) = \frac{1}{2}p^2 - \cos q$$



so that the equation of motion read

$$\begin{cases} d_t p = -\sin q \\ d_t q = p \end{cases}$$

and we refer to PC2 for a representation of the orbits in the phase space. (See also the Figure Page 10).

Remark: We refer to the Lectures Notes of E. HAIRER for the Kepler Problem and for Hénon-Heiles problem for a Hamiltonian dynamical system, which can generate chaos.

II.3 Symplectic transformations.

We introduce in this subsection the proper notion we will want our numerical scheme to mimic while integrating Hamiltonian dynamical systems. The basic objects to be studied are two dimensional parallelograms lying in $\mathbb{R}^{2d}$, defined by two vectors in $\mathbb{R}^{2d}$

$$\xi = \begin{pmatrix} \xi^p \\ \xi^q \end{pmatrix} \qquad \eta = \begin{pmatrix} \eta^p \\ \eta^q \end{pmatrix}$$

in the space of (p,q), $(\xi^p, \xi^q, \eta^p, \eta^q \in \mathbb{R}^d)$
as

$$P = \{ t\xi + s\eta \mid 0 \le t \le 1, \ 0 \le s \le 1 \}.$$

In the case $d=1$, we consider the oriented area

$$\text{or.area}(P) = \det \begin{vmatrix} \xi^p & \eta^p \\ \xi^q & \eta^q \end{vmatrix} = \xi^p \eta^q - \xi^q \eta^p$$

In higher dimensions, we replace this with the sum of the oriented areas of the projection of P onto the coordinates (p_i, q_i)

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

This defines a bilinear mapping acting on vectors of $\mathbb{R}^{2d}$, which plays a central role in the study of Hamiltonian Systems.

Using matrix notations:

(10) $$\omega(\xi,\eta) = \xi^t J \eta \quad \text{with} \quad J = \begin{pmatrix} 0 & +\mathbb{I}_{\mathbb{R}^d} \\ -\mathbb{I}_{\mathbb{R}^d} & 0 \end{pmatrix}$$

where $\mathbb{I}_{\mathbb{R}^d}$ is the identity matrix in $\mathbb{R}^d$.

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

(11) if $$A^t J A = J \quad \text{or equivalently} \quad \omega(\xi,\eta) = \omega(A\xi, A\eta) \quad \forall (\xi,\eta) \in \mathbb{R}^{2d}$$

In the specific case $d=1$, where $\omega(\xi,\eta)$ represent the area of parallelogram P symplecticity means that the linear mapping is area preserving.

Definition: A differential map: $g: U \to \mathbb{R}^{2d}$ (U open set, $U \subset \mathbb{R}^{2d}$) is called symplectic if the Jacobian matrix $A = \partial_{p,q}\, g(p,q)$ is everywhere symplectic,

$$A^t J A = J \quad \text{or} \quad \omega(A\xi, A\eta) = \omega(\xi, A\eta) \quad \forall (\xi,\eta) \in U. \tag{12}$$

These notions are essential in order to present the principal result of this theoretical section: Let us take $y = \begin{pmatrix} p \\ q \end{pmatrix} \in \mathbb{R}^{2d}$ and write the dynamical system of Hamiltonian type (canonical form).

$$d_t y = J^{-1} (\partial_y H)^t \tag{13}$$

where $J = \begin{pmatrix} 0 & I_{\mathbb{R}^d} \\ -I_{\mathbb{R}^d} & 0 \end{pmatrix}$, and where φ_t is the flow

$\varphi_t(p_0,q_0) = \begin{pmatrix} p(t,p_0,q_0) \\ q(t,p_0,q_0) \end{pmatrix}$ with initial values $\begin{pmatrix} p_0 \\ q_0 \end{pmatrix} \in \mathbb{R}^{2d}$.

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 φ_t is a symplectic transformation wherever it is defined.

PROOF : The derivative $\partial_{y_0}\varphi_t$ at $t=0$ is the identity and satisfies the variational equation for the solution of the Hamiltonian system (13)

$$d_t\Psi = J^{-1}\partial_{yy}H(\varphi_t(y_0))\Psi$$

where $\partial_{yy}H$ is the Hessian matrix related to the Hamiltonian and is therefore symmetric.

F/t $t=0$. we have $$\left(\partial_{y_0}\varphi_t\right)^t J\, \partial_{y_0}\varphi_t = J$$

since $\partial_{y_0}\varphi_t$ at $t=0$ is the identity matrix.

Let us write a dynamical system on this quantity.

$$d_t\left(\left(\partial_{y_0}\varphi_t\right)^t J\,\partial_{y_0}\varphi_t\right) = d_t\left(\partial_{y_0}\varphi_t\right)^t J\,\partial_y\varphi_t + \left(\partial_{y_0}\varphi_t\right)^t J\, d_t\left(\partial_y\varphi_t\right)$$

$$= \left(\partial_{y_0}\varphi_t\right)^t \partial_{yy}H(\varphi_t(y_0))\left(J^{-1}\right)^t J\left(\partial_y\varphi_t\right)$$

$$+ \left(\partial_y\varphi_t\right)^t J J^{-1}\partial_{yy}H(\varphi_t(y_0))\,\partial_y\varphi_t = 0$$

Since $J^t = -J \Rightarrow \left(J^{-1}\right)^t J = -\mathrm{Id}_{\mathbb{R}^{2d}}$

Thus,

$$\left(\partial_{y_0}\varphi(t)\right)^t J\,\partial_{y_0}\varphi(t) = J \quad \forall t$$ as long as the solution remain in the domain of definition of H.

$\square$

We illustrate this theorem with the pendulum $H(p,q) = \frac{p^2}{2} - \cos q$
The Figure shows level curves of the total energy and also illustrate the area preservation of the flow φ_t. The areas of A and B and of $\varphi_t(A)$ and $\varphi_t(B)$ are the same even if their appearances have changed completely.

In fact symplecticity is a characteristic property of dynamical systems of Hamiltonian type.

THEOREM: We call a dynamical system $d_t y = f(y)$ locally Hamiltonian if $\forall y_0 \in U$, $\exists$ a neighborhood of y_0 such that $f(y) = J^{-1} (\partial_y H)^T$ for some function H. If f is continuously differentiable, then $d_t y = f(y)$ is locally Hamiltonian if and only if $\varphi_t(y)$ is symplectic $\forall y \in U$ and for all sufficiently small t.

PROOF: See HAIRER Lecture Notes. □

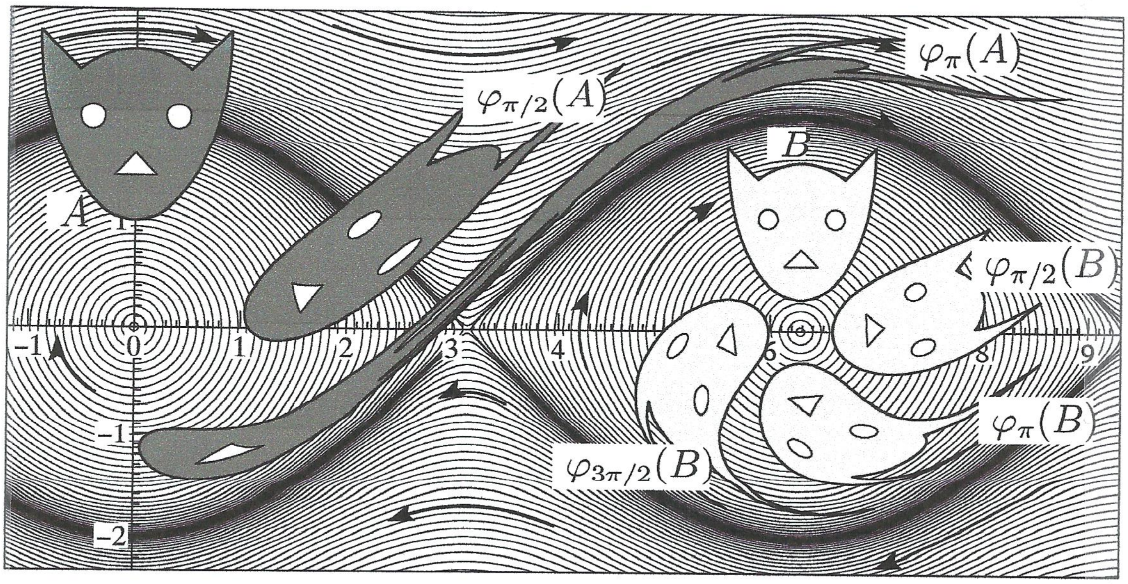


Figure Area preservation of the flow of Hamiltonian systems

Remark: Hamiltonian systems are then directly related to symplectic mappings. Let us underline that the form of the Hamiltonian system in (13) is given with a specific matrix J, which is called "canonical". We will see that Hamiltonian systems can be generalized without altering their geometric properties, in particular, we may allow J to be any invertible constant skew-symmetric matrix $J^t = -J$. (See Leimkuhler and Reich. 2004 - HAIRER-LUBICH-WANNER).

II.4 Generating functions

Whereas Hamiltonian systems are described by a single scalar function, the Hamiltonian, symplectic mappings can be described by one scalar function called the generating function. The results are conveniently formulated in terms of differential forms. For the function $F(y)$ $dF = dF(y)$ is its Fréchet derivative, that is the linear mapping:

$$dF(y)(\xi) = \partial_y F(y)\, \xi = \sum_{i=1}^{n} \partial_{y_i} F\, \xi_i$$

For the special case $F(y) = y_k$, we denote the derivative dy_k so that $dy_k(\xi) = \xi_k$ is the projection on the kth component. With $dy = (dy_1 - dy_k)^t$ we have $dF = \sum_{i=1}^{n} \partial_y F\, dy_i$

For a function $S(p,q)$ it yields

$$dS(p,q) = dS = S_p\,dp + S_q\,dq = \sum_{i=1}^{d} \left(\partial_{p_i} S(p,q)\,dp_i + \partial_{q_i} S(p,q)\,dq_i\right)$$

where S_p and S_q are now vectors of partial derivative and

$$dp = (dp_1 - dp_d)^t, \quad dq = (dq_1 - dq_d)^t$$

THEOREM: A mapping $\varphi : (p,q) \mapsto (P,Q)$ is symplectic if and only if there exists locally a function $S(p,q)$ such that

$$(14) \qquad P^t dQ - p^t dq = dS$$

This means that $P^t dQ - p^t dq$ is a total differential.

PROOF: We use the following notation for the Jacobian.

$$\frac{\partial(P,Q)}{\partial(p,q)} = \begin{pmatrix} P_p & P_q \\ Q_p & Q_q \end{pmatrix}$$

we thus have $\begin{pmatrix} P_p & P_q \\ Q_p & Q_q \end{pmatrix}^t J \begin{pmatrix} P_p & P_q \\ Q_p & Q_q \end{pmatrix} = J$

which yields three conditions

$$(15) \left\{ \begin{array}{ll} P_p^t Q_p = Q_p^t P_p & P_p^t Q_p - I = Q_p^t P_q \\ & Q_q^t P_q = P_q^t Q_q \end{array} \right.$$

equivalent to symplecticity. We now insert $dQ = Q_p\,dp + Q_q\,dq$ in (14) and obtain

$$\left(P^t Q_p,\ P^t Q_q - p^t\right)\begin{pmatrix} dp \\ dq \end{pmatrix} = \begin{pmatrix} Q_p^t P \\ Q_q^t P - p \end{pmatrix}^t \begin{pmatrix} dp \\ dq \end{pmatrix}$$

In order to apply the integrability lemma (given below), we have to verify the symmetry of the Jacobian of the coefficient vector:

$$(16)\quad \begin{pmatrix} Q_p^t P_p & Q_p^t P_q \\ Q_q^t P_p - I & Q_q^t P_q \end{pmatrix} + \sum_i P_i \underbrace{\frac{\partial^2 Q_i}{\partial(p,q)^2}}_{\text{symmetric.}}$$

It is clear that matrix (16) symmetric is equivalent to (15).

∎

<u>Lemma of integrability</u>. $D \subset \mathbb{R}^n$ an open set

$f: D \to \mathbb{R}^n$ continuously differentiable such that the Jacobian matrix is symmetric $\partial_y f(y)$ $\forall y \in D$.
Then for every $y_0 \in D$, $\exists$ a neighborhood and a function $H(y)$ such that $f(y) = (\partial_y H)^t$

PROOF. See HAIRER - Cours □

Relation (14) tends to show that the most convenient choice of variables for the mapping S is (q, Q). When working with mappings close to identity, such as for numerical integrators, it is more convenient to use <u>mixed variables</u> such as (P, q), (p, Q) or $((P+p)/2, (Q+q)/2)$.

THEOREM: Let $(p,q) \mapsto (P,Q)$ be a smooth transformation close to identity. It is symplectic if and only if one of the following conditions locally holds:

- $Q^t dP + p^t dq = d(P^t q + S^1)$ for some function $S^1(P,q)$
- $P^t dQ + q^t dp = d(p^t Q - S^2)$ — — — — $S^2(p,Q)$
- $(Q-q)^t d(P+p) - (P-p)^t d(Q+q) = 2\, dS^3$

  for some function $S^3\left(\frac{P+p}{2}, \frac{Q+q}{2}\right)$.

The generating functions S^1, S^2 and S^3 have been chosen such that we obtain the identity mapping when they are replaced with zero. Comparing the coefficients functions of dq and dP in the first line above, we obtain:

$$(17) \begin{cases} p = P + \partial_q S^1(P,q) \\ Q = q + \partial_P S^1(P,q) \end{cases}$$

whatever the scalar function S^1, relation (17) defines a symplectic transformation $(p,q) \mapsto (P,Q)$.
Similar relations can be derived for the other two relations.

From these results, a direct link between a Hamiltonian system and the generating function can be made through the Hamilton-Jacobi partial differential equation and we refer to the Lecture Notes of HAIRER – TUM. 2009/10.