## Lecture 1: Some basics

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Numerical methods for ODEs

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- What is a differential equation ?
- Some methods of resolution:
  - Separation of variables;
  - Change of variables;
  - Method of integrating factors.
- Important examples of ODEs:
  - Autonomous ODEs;
  - Exact equations;
  - Hamiltonian systems.

- Ordinary differential equation (ODE): equation that contains one or more derivatives of an unknown function x(t).
- Equation may also contain x itself and constants.
- ODE of order *n* if the *n*-th derivative of the unknown function is the highest order derivative in the equation.

- Examples of ODEs:
  - Membrane equation as a neuron model:

$$C\frac{dx(t)}{dt}+gx(t)=f(t),$$

x(t): membrane potential, i.e., the voltage difference between the inside and the outside of the neuron; f(t): current flow due to excitation; C: capacitance; g: conductance (the inverse of the resistance) of the membrane.

• Linear ODE of order 1.

• Theta model: one-dimensional model for the spiking of a neuron.

$$rac{d heta(t)}{dt} = 1 - \cos heta(t) + (1 + \cos heta(t))f(t);$$

f(t): inputs to the model.

- $\theta \in [0, 2\pi]$ ;  $\theta = \pi$  the neuron spikes  $\rightarrow$  produces an action potential.
- Change of variables, x(t) = tan(θ(t)/2), → quadratic model

$$(*) \quad \frac{dx(t)}{dt} = x^2(t) + f(t).$$

Population growth under competition for resources:

$$(**) \quad \frac{dx(t)}{dt} = rx(t) - \frac{r}{k}x^2(t);$$

*r* and *k*: positive parameters; x(t): number of cells at time instant *t*, rx(t): growth rate and  $-(r/k)x^2(t)$ : death rate.

• (\*) and (\*\*): Nonlinear ODEs of order 1.

• FitzHugh-Nagumo model:

$$\frac{dV}{dt} = f(V) - W + I,$$
$$\frac{dW}{dt} = a(V - bW);$$

- V: membrane potential, W: recovery variable, and I: magnitude of stimulus current.
- f(V): polynomial of third degree, and a and b: constant parameters.
- FitzHugh-Nagumo model: two-dimensional simplification of the Hodgkin-Huxley model of spike generation in squid giant axons.
- Mathematical properties of excitation and propagation from the electrochemical properties of sodium and potassium ion flow.
- System of nonlinear ODEs of order 1.

• Langevin equation of motion for a single particle:

$$rac{dx(t)}{dt} = -ax(t) + \eta(t);$$

- x(t): position of the particle at time instant t, a > 0: coefficient of friction, and η: random variable that represents some uncertainties or stochastic effects perturbing the particle.
- Diffusion-like motion from the probabilistic perspective of a single microscopic particle moving in a fluid medium.
- Linear stochastic ODE of order 1.

• Vander der Pol equation:

$$rac{d^2 x(t)}{dt^2} - a(1-x^2(t)) rac{dx(t)}{dt} + x(t) = 0;$$

- *a*: positive parameter, which controls the nonlinearity and the strength of the damping.
- Generate waveforms corresponding to electrocardiogram patterns.
- Nonlinear ODE of order 2.

- Higher order ODEs:  $\Omega \subset \mathbb{R}^{n+2}$  and  $n \in \mathbb{N}$ .
- ODE of order *n*:

$$F(t,x(t),\frac{dx}{dt}(t),...,\frac{d^nx}{dt^n}(t))=0;$$

- x: real-valued unknown function and dx(t)/dt,..., d<sup>n</sup>x(t)/dt<sup>n</sup>: its derivatives.
- φ ∈ C<sup>n</sup>(I): solution of the differential equation if I: open interval, for all t ∈ I,

$$(t, arphi(t), rac{\partial arphi}{\partial t}(t), ..., rac{\partial^n arphi}{\partial t^n}(t)) \in \Omega$$

and

$$F(t, \varphi(t), \frac{\partial \varphi}{\partial t}(t), ..., \frac{\partial^n \varphi}{\partial t^n}(t)) = 0.$$

• x: vector valued function,  $x(t) \in \mathbb{R}^d$ ,  $\to \Omega \subset \mathbb{R} \times \mathbb{R}^{(n+1)d}$ .

• *n*-th order ODE:

$$(***)$$
  $x^{(n)}(t) = f(t, x, \frac{dx}{dt}, ..., \frac{d^{n-1}x}{dt^{n-1}}), t \in I.$ 

- $x(t) \in \mathbb{R}^d$  and  $f: I \times \mathbb{R}^{nd} \to \mathbb{R}^d$ .
- Initial condition:

$$(x(t_0), x'(t_0), x''(t_0), ..., x^{(n-1)}(t_0))^{\top}.$$

• Reduce the high order ODE (\* \* \*) into a first order ODE:

$$y(t) := (x(t), dx(t)/dt, ..., d^{n-1}x(t)/dt^{n-1})^{\top} \in \mathbb{R}^{nd}$$

and

$$F(t, y) := (y_2, ..., y_n, f(t, y_1, ..., y_n))^{\top}$$
  
for  $y = (y_1, ..., y_n)^{\top} \in \mathbb{R}^{nd}$  and  $y_i \in \mathbb{R}^d$  for  $i = 1, 2, ..., n$ 

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• (\* \* \*) equivalent to the following first order ODE:

$$\frac{dy}{dt}=F(t,y(t)).$$

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- EXAMPLE:
  - Consider the second order ODE:

$$\frac{d^2x}{dt^2} + p(t)\frac{dx}{dt} + q(t)x(t) = g(t).$$

•  $\Rightarrow$ 

$$\frac{d}{dt} \begin{bmatrix} x \\ \frac{dx}{dt} \end{bmatrix} = \begin{bmatrix} \frac{dx}{dt} \\ -p(t)\frac{dx}{dt} - q(t)x(t) + g(t) \end{bmatrix}$$
$$= \begin{bmatrix} 0 & 1 \\ -q(t) & -p(t) \end{bmatrix} \begin{bmatrix} x \\ \frac{dx}{dt} \end{bmatrix} + \begin{bmatrix} 0 \\ g(t) \end{bmatrix}.$$

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#### • ODEs:

- Existence of solutions;
- Uniqueness of solutions with suitable initial conditions;
- Regularity and stability of solutions (e.g. dependence on the initial conditions, large time stability, higher regularity);
- Computation of solutions.
- Existence of solutions: fixed point theorems; implicit function theorem in Banach spaces.
- Uniqueness: more difficult.
- Explicit solutions: only in a very few special cases.
- Numerical solutions.

- Some methods of resolution:
  - Separation of variables;
  - Change of variables;
  - Method of integrating factors.

- Separation of variables:
  - I and J: open intervals;
  - $f \in C^0(I)$  and  $g \in C^0(J)$ : continuous functions.
  - Solutions to the first order equation

$$(****)\quad \frac{dx}{dt}=f(t)g(x).$$

- $t_0 \in I$  and  $x_0 \in J$ ; initial condition:  $x(t_0) = x_0$ .
- $g(x_0) = 0$  for some  $x_0 \in J \rightarrow x(t) = x_0$  for  $t \in I$ : solution to (\* \* \*\*).
- Suppose  $g(x_0) 
  eq 0 
  ightarrow g 
  eq 0$  in a neighborhood of  $x_0 \Rightarrow$

$$\frac{dx}{g(x)}=f(t)dt.$$

• Integration  $\Rightarrow$ 

$$\int \frac{dx}{g(x)} = \int f(t)dt + c;$$

c: constant uniquely determined by the initial condition.

- F and G: primitives of f and 1/g.
- $G'(x) \neq 0 \Rightarrow G$ : strictly monotonic  $\rightarrow$  invertible.
- Solution:

$$x(t) = G^{-1}(F(t) + c).$$

- Method of separation of variables.
- (\* \* \*\*): separable equation.

- EXAMPLE:
  - Consider the following ODE:

$$\begin{cases} \frac{dx}{dt} = \frac{1+2t}{\cos x(t)}, \\ x(0) = \pi. \end{cases}$$

- $g(x) = 1/\cos x$  and f(t) = 1 + 2t.
- g: defined for  $x \neq \pi/2 + k\pi, k \in \mathbb{Z}$ .
- Separation of variables,

$$\cos x dx = (1+2t) dt.$$

• Integration,

$$\sin x(t) = t^2 + t + C,$$

for some constant  $C \in \mathbb{R}$ .

• Initial condition  $x(0) = \pi \Rightarrow C = 0$ .

- Taking the  $\arcsin \Rightarrow x(t) = \arcsin(t^2 + t)$ : not the solution because  $x(0) = \arcsin(0) = 0$ .
- arcsin: inverse of sin on [-π/2, π/2]; x(t): takes the values in a neighborhood of π.

• 
$$w(t) = x(t) - \pi \rightarrow w(0) = x(0) - \pi = 0 \Rightarrow w(t) = -\arcsin(t^2 + t).$$

• Correct solution:

$$x(t) = \pi - \arcsin(t^2 + t).$$

- Change of variables:
  - Consider the following ODE:

$$\frac{dx}{dt} = f\left(\frac{x(t)}{t}\right);$$

 $f: I \subset \mathbb{R} \to \mathbb{R}$ : continuous function on some open interval  $I \subset \mathbb{R}$ .

• change of variable x(t) = ty(t); y(t): new unknown function,

$$\frac{dx}{dt} = y(t) + t\frac{dy}{dt} = f(y(t)),$$

• Separable equation for *y*:

$$\frac{dy}{f(y)-y}=\frac{dt}{t}.$$

• Solution by the method of separation of variables.

• EXAMPLE:

•  $\Rightarrow$ 

Consider

$$\frac{dx}{dt} = \frac{t^2 + x^2}{xt}.$$

• 
$$f(s) = s + 1/s$$
 with  $s = x/t$ .

• Change of variable:  $y(t) = x(t)/t \Rightarrow ydy = dt/t$ 

$$(1/2)y^2 = \ln t + C.$$

$$\Rightarrow x(t) = \pm t \sqrt{2(\ln t + C)}.$$

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- Method of integrating factors
  - Consider

$$\frac{dx(t)}{dt}=f(t).$$

• Integration

$$x(t)=x(0)+\int_0^t f(s)\,ds.$$

• Consider

$$\frac{dx}{dt} + p(t)x(t) = g(t);$$

p and g: functions of t.

• Left-hand side: expressed as the derivative of the unknown quantity  $\leftarrow$  Multiply by  $\mu(t)$ .

•  $\mu(t)$  s.t.

$$\mu(t)\frac{dx}{dt} + \mu(t)p(t)x(t) = \frac{d}{dt}(\mu(t)x(t)).$$

• Taking derivatives  $\Rightarrow$ 

$$(1/\mu)d\mu/dt = p(t)$$
 or  $\frac{d}{dt}\ln\mu(t) = p(t).$ 

• Integration  $\Rightarrow$ 

$$\mu(t) = \exp(\int_0^t p(s)ds),$$

up to a multiplicative constant.

• Transformed equation:

$$\frac{d}{dt}(\mu(t)x(t)) = \mu(t)g(t).$$

 $\bullet \Rightarrow$ 

$$x(t) = \frac{1}{\mu(t)} \left( \int_0^t \mu(s)g(s)ds \right) + \frac{C}{\mu(t)};$$

C: determined from the initial condition  $x(0) = x_0$ .

•  $\mu(t)$ : integrating factor.

- EXAMPLE:
  - Consider

$$\begin{cases} \frac{dx}{dt} + \frac{1}{t+1}x(t) = (1+t)^2, & t \ge 0, \\ x(0) = 1. \end{cases}$$

• 
$$p(t) = 1/(t+1)$$
 and  $g(t) = (1+t)^2$ .

• Integrating factor:

$$\mu(t) = \exp(\int_0^t p(s)ds) = e^{\ln(t+1)} = t+1.$$

 $\bullet \Rightarrow$ 

$$x(t) = rac{1}{t+1} \int_0^t (s+1)^3 ds + rac{C}{t+1} = rac{(t+1)^3}{4} + rac{C-rac{1}{4}}{t+1}$$

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• Initial condition  $x(0) = 1 \Rightarrow C = 1$ .

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- EXAMPLE: (Bernoulli's equation)
  - Consider

$$\frac{dx}{dt} + p(t)x(t) = g(t)x^{\alpha}(t).$$

- $\alpha \notin \{0,1\}.$
- Change of variable:  $x = z^{\frac{1}{1-\alpha}}$ ,

$$\frac{dx}{dt} = \frac{1}{1-\alpha} z^{\frac{\alpha}{1-\alpha}} \frac{dz}{dt}.$$

• Linear equation:

$$\frac{dz}{dt} + (1-\alpha)p(t)z(t) = (1-\alpha)g(t).$$

• Solved by the method of integrating factors.

- Important examples of ODEs:
  - Autonomous ODEs;
  - Exact equations;
  - Hamiltonian systems.

- Autonomous ODEs:
  - DEFINITION:  $\frac{dx(t)}{dt} = f(t, x(t))$ : autonomous if f: independent of t.
  - Any ODE can be rewritten as an autonomous ODE on a higher-dimensional space.
  - $y = (t, x(t)) \rightarrow$  autonomous ODE

$$\frac{dy(t)}{dt} = F(y(t));$$

$$F(y) = \begin{pmatrix} 1 \\ f(t, x(t)) \end{pmatrix}.$$

- Exact equations:
  - $\Omega = I \times \mathbb{R} \subset \mathbb{R}^2$  with  $I \subset \mathbb{R}$ : open interval.
  - $f,g \in C^0(\Omega)$ .
  - Solution  $x \in C^1(I)$  of the ODE:

$$f(t,x(t)) + g(t,x(t))\frac{\mathrm{d}x}{\mathrm{d}t} = 0$$

satisfying the initial condition  $x(t_0) = x_0$  for some  $(t_0, x_0) \in \Omega$ .

• Differential form:

$$\omega = f(t, x) \mathrm{d}t + g(t, x) \mathrm{d}x.$$

DEFINITION: Differential form: exact if there exists
 F ∈ C<sup>1</sup>(Ω) s.t.

$$\omega = \mathrm{d}F = \frac{\partial F}{\partial t}\mathrm{d}t + \frac{\partial F}{\partial x}\mathrm{d}x.$$

- F: potential of  $\omega$ .
- Differential equation: exact equation.

- THEOREM: Implicit function theorem
  - Suppose that F(t, x): continuously differentiable in a neighborhood of (t<sub>0</sub>, x<sub>0</sub>) ∈ ℝ × ℝ<sup>d</sup> and F(t<sub>0</sub>, x<sub>0</sub>) = 0.
  - Suppose that  $\partial F/\partial x(t_0, x_0) \neq 0$ .
  - Then there exists a  $\delta > 0$  and  $\epsilon > 0$  s.t. for each t satisfying  $|t t_0| < \delta$ , there exists a unique x s.t.  $|x x_0| < \epsilon$  for which F(t, x) = 0.
  - This correspondence defines a function x(t) continuously differentiable on {|t − t<sub>0</sub>| < δ} s.t.</li>

$$F(t,x)=0 \Leftrightarrow x=x(t).$$

- THEOREM:
  - Suppose that  $\omega$ : exact form with potential F s.t.

$$\frac{\partial F}{\partial x}(t_0,x_0)\neq 0.$$

F(t,x) = F(t<sub>0</sub>, x<sub>0</sub>) implicitly defines a function x ∈ C<sup>1</sup>(I) for some open interval I containing t<sub>0</sub>, which solves

$$f(t,x(t)) + g(t,x(t))\frac{\mathrm{d}x}{\mathrm{d}t} = 0$$

with the initial condition  $x(t_0) = x_0$ .

• Solution: unique on *I*.

- PROOF:
  - Suppose without loss of generality that  $F(t_0, x_0) = 0$ .
  - Implicit function theorem  $\Rightarrow$  there exists  $\delta, \eta > 0$  and  $x \in C^1(t_0 \delta, t_0 + \delta)$  s.t.  $\{(t, x) \in \Omega : |t - t_0| < \delta, |x - x_0| < \eta,$  $F(t, x) = 0\} = \{(t, x(t)) \in \Omega : |t - t_0| < \delta\}.$
  - By differentiating the identity F(t, x(t)) = 0,

$$\begin{aligned} 0 &= \frac{\mathrm{d}}{\mathrm{d}t} F(t, x(t)) &= \frac{\partial F}{\partial t}(t, x(t)) + \frac{\partial F}{\partial x}(t, x(t)) \frac{\mathrm{d}x}{\mathrm{d}t} \\ &= f(t, x(t)) + g(t, x(t)) \frac{\mathrm{d}x}{\mathrm{d}t}. \end{aligned}$$

•  $\Rightarrow x(t)$ : solution of the differential equation.

• 
$$x(t_0) = x_0$$

• If  $z \in \mathcal{C}^1(I)$ : solution s.t.  $z(t_0) = x_0$ , then

$$\frac{\mathrm{d}}{\mathrm{d}t}F(t,z(t))=0\Longrightarrow F(t,z(t))=F(t_0,z(t_0))=0\Longrightarrow z(t)=x(t).$$

- DEFINITION:
  - $f,g \in \mathcal{C}^1(\Omega)$ .
  - Differential form  $\omega = f dt + g dx$ : closed in  $\Omega$  if

$$\frac{\partial f}{\partial x} = \frac{\partial g}{\partial t}$$

for all  $(t, x) \in \Omega$ .

- PROPOSITION:
  - Exact differential form ω = f dt + g dx with a potential F ∈ C<sup>2</sup>: closed since

$$\frac{\partial^2 F}{\partial t \partial x} = \frac{\partial^2 F}{\partial x \partial t}$$

for all  $(t, x) \in \Omega$ .

- Converse: also true if  $\Omega$ : simply connected.
- Closed forms always have a potential (at least locally).

- EXAMPLE:
  - Consider

$$tx^2 + x - t\frac{\mathrm{d}x}{\mathrm{d}t} = 0.$$

- $f(t,x) = tx^2 + x$  and g(t,x) = -t.
- Not exact:

$$\frac{\partial f}{\partial x} = 2xt + 1 \neq \frac{\partial g}{\partial t} = -1.$$

- EXAMPLE:
  - Consider

$$t + \frac{1}{x} - \frac{t}{x^2} \frac{\mathrm{d}x}{\mathrm{d}t} = 0$$

• Exact equation with the potential function *F*:

$$F(t,x) = rac{t^2}{2} + rac{t}{x} + C, \quad C \in \mathbb{R}$$

F(t,x) = 0 implicitly defines the solutions (locally for t ≠ 0 and x ≠ 0 s.t. ∂F/∂x(t,x) ≠ 0).

- Hamiltonian systems:
  - DEFINITION:
    - *M*: subset of  $\mathbb{R}^d$  and  $H : \mathbb{R}^d \times M \to \mathbb{R}$ :  $\mathcal{C}^1$  function.
    - Hamiltonian system with Hamiltonian *H*: first-order system of ODEs

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

- 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, widely used Hamiltonian systems in molecular dynamics: H(p,q) = ½p<sup>T</sup>M<sup>-1</sup>p + V(q); M: symmetric positive definite matrix and ⊤: transpose.

- Invariant for a system of ODEs:
  - DEFINITION:
    - $\Omega = I \times D$ ;  $I \subset \mathbb{R}$  and  $D \subset \mathbb{R}^d$ .
    - Consider

$$\frac{\mathrm{d}x}{\mathrm{d}t}=f(t,x(t));$$

- $f: \Omega \to \mathbb{R}^d$ .
- $F: D \to \mathbb{R}$ : invariant if F(x(t)) = Constant.
- $(t,x) \in I \times D$ : stationary point if f(t,x) = 0.

- Example:
  - Lotka-Volterra's ODEs:

$$\begin{cases} \frac{\mathrm{d}u}{\mathrm{d}t} = u(v-2),\\ \frac{\mathrm{d}v}{\mathrm{d}t} = v(1-u). \end{cases}$$

- Dynamics of biological systems in which two species interact: one as a predator and the other as prey.
- Define

$$F(u,v) := \ln u - u + 2 \ln v - v.$$

- F(u, v): invariant.
- (u, v) = (1, 2) and (u, v) = (0, 0): stationary points.

• Differentiation with respect to time,

$$\frac{d}{dt}F(u,v) = \frac{1}{u}\frac{du}{dt} - \frac{du}{dt} + \frac{2}{v}\frac{dv}{dt} - \frac{dv}{dt}$$
  
=  $v - 2 - \frac{du}{dt} + 2(1-u) - \frac{dv}{dt}$   
=  $(v-2) - u(v-2) + 2(1-u) + v(1-u)$   
=  $(v-2)(1-u) + (2-v)(1-u)$   
=  $0.$ 

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- LEMMA:
  - Hamiltonian *H*: invariant of the associated Hamiltonian system.
- PROOF:

• 
$$\frac{\mathrm{d}}{\mathrm{d}t}H(p(t),q(t))$$

$$= \frac{\partial H}{\partial p}(p(t),q(t))\frac{\mathrm{d}p}{\mathrm{d}t} + \frac{\partial H}{\partial q}(p(t),q(t))\frac{\mathrm{d}q}{\mathrm{d}t}$$

$$= -\frac{\partial H}{\partial p}(p(t),q(t))\frac{\partial H}{\partial q}(p(t),q(t)) + \frac{\partial H}{\partial q}(p(t),q(t))\frac{\partial H}{\partial p}(p(t),q(t))$$

$$= 0.$$

• H(p,q): invariant of the associated system of equations.

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- EXAMPLE:
  - Consider

$$\begin{cases} \frac{\mathrm{d}p}{\mathrm{d}t} = -\sin q, \\ \frac{\mathrm{d}q}{\mathrm{d}t} = p. \end{cases}$$

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

$$\begin{cases} \frac{\partial H}{\partial q} = \sin q = -\frac{\mathrm{d}p}{\mathrm{d}t},\\ \frac{\partial H}{\partial p} = p = \frac{\mathrm{d}q}{\mathrm{d}t}. \end{cases}$$

• 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

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

- Notation  $\nabla H(x) := \left(\frac{\partial H}{\partial x}\right)^{\top} = \left(\frac{\partial H}{\partial x_1}, \dots, \frac{\partial H}{\partial x_{2d}}\right)^{\top}$ .
- For a vector function  $f : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ ,  $f(x) = (f_1(x), \dots, f_{2d}(x))$ , we define the Jacobian matrix f' of f by

$$f'(x) := \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_{2d}} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_{2d}}{\partial x_1} & \cdots & \frac{\partial f_{2d}}{\partial x_{2d}} \end{pmatrix}$$

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- 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  $A^{\top}JA = J$ .

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- DEFINITION Symplectic mapping
  - Differentiable map g : U → ℝ<sup>2d</sup>: symplectic if the Jacobian matrix g'(p, q): everywhere symplectic, i.e., if

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

• Taking the transpose of both sides of the above equation,

$$g'(p,q)^{\top}J^{\top}g'(p,q)=J^{\top};$$

• Or equivalently,

 $g'(p,q)^{\top}J^{-1}g'(p,q) = J^{-1}.$ 

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

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• PROOF:

• 
$$x = (p, q)^{\top}, y = g(p, q)^{\top}; G(y) := H(x).$$

• Chain rule 
$$\Rightarrow$$

$$\frac{\partial}{\partial x}H(x) = \frac{\partial}{\partial x}G(y) = \frac{\partial}{\partial y}G(y)\frac{\partial y}{\partial x}(x)$$
$$= (\nabla_y G(y))^\top g'^\top (p,q).$$

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$$\begin{split} \frac{\mathrm{d}y}{\mathrm{d}t} &= g'^{\top}(p,q)\frac{\mathrm{d}x}{\mathrm{d}t} \\ &= g'^{\top}(p,q)J^{-1}\left(\frac{\partial H(x)}{\partial x}\right)^{\top} \\ &= g'^{\top}J^{-1}g'\nabla_{y}G(y) \\ &= J^{-1}\nabla_{y}G(y). \\ &\qquad \frac{\mathrm{d}y}{\mathrm{d}t} = J^{-1}\nabla_{y}G(y). \end{split}$$

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- DEFINITION:
  - Flow:

 $\phi_t(p_0,q_0) = x(t,p_0,q_0) = (p(t,p_0,q_0),q(t,p_0,q_0))^{\top};$ 

• 
$$\phi_t: U \to \mathbb{R}^{2d}, \ U \subset \mathbb{R}^{2d};$$

•  $p_0$  and  $q_0$ : initial data at t = 0.

• 
$$y_0 = (p_0, q_0)^{\top}; f = J^{-1} \nabla H$$
:

$$\frac{d\phi_t(y_0)}{dt} = f(\phi_t(y_0)) \Rightarrow \frac{d}{dt} \frac{\partial\phi_t(y_0)}{\partial y_0} = f'(\phi_t(y_0)) \frac{\partial\phi_t(y_0)}{\partial y_0};$$
$$f' = J^{-1} \nabla^2 H,$$

•  $\nabla^2 H$ : Hessian matrix of H

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- THEOREM: Poincaré's theorem
  - *H*: twice differentiable.
  - Flow  $\phi_t$ : symplectic transformation.

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• PROOF:

$$y_{0} = (p_{0}, q_{0})^{\top}.$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \left( \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right)^{\top} J \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right) \right)$$

$$= \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right)^{\prime^{\top}} J \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right) + \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right)^{\top} J \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right)^{\prime}$$

$$= \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right)^{\top} \nabla^{2} H J^{-\top} J \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right) + \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right)^{\top} J J^{-1} \nabla^{2} H \left( \frac{\partial \phi_{t}}{\partial y_{0}} \right)$$

$$= 0;$$

• Hessian matrix  $\nabla^2 H$  of H(p,q): symmetric.

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•  $\partial \phi_t / \partial y_0$  at t = 0: identity map  $\Rightarrow$ 

$$\left(\frac{\partial \phi_t}{\partial y_0}\right)^\top J\left(\frac{\partial \phi_t}{\partial y_0}\right) = J$$

for all t and all  $(p_0, q_0)$ .

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

- PROOF:
  - Necessity  $\Leftarrow$  Poincaré's Theorem.
  - Suppose that  $\phi_t$ : symplectic; prove local existence of a Hamiltonian H s.t.  $f(x) = J^{-1} \nabla H(x)$ .
  - $\frac{\partial \phi_t}{\partial y_0}$ : solution of

$$\frac{\mathrm{d}y}{\mathrm{d}t} = f'(\phi_t(y_0))y;$$

•  $\Rightarrow$ 

$$\frac{\mathrm{d}}{\mathrm{d}t} \left( \left( \frac{\partial \phi_t}{\partial y_0} \right)^\top J \left( \frac{\partial \phi_t}{\partial y_0} \right) \right) = \left( \frac{\partial \phi_t}{\partial y_0} \right)^\top [f'(\phi_t(y_0))^\top J + Jf'] \left( \frac{\partial \phi_t}{\partial y_0} \right)$$
$$= 0.$$

- Putting t = 0;  $J = -J^{\top} \Rightarrow Jf'(y_0)$ : symmetric matrix for all  $y_0$ .
- Integrability lemma  $\Rightarrow$  Jf(y): can be written as the gradient of a function H.

- LEMMA: Integrability lemma
  - $D \subset \mathbb{R}^{2d}$ : open set;  $g : D \to \mathbb{R}^{2d} \in \mathcal{C}^1$ .
  - Suppose that the Jacobian g'(y): symmetric for all  $y \in D$ .
  - For every y<sub>0</sub> ∈ D, there exists a neighborhood of y<sub>0</sub> and a function H(y) s.t.

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

on this neighborhood.

- PROOF:
  - Suppose that  $y_0 = 0$ , and consider a ball around  $y_0$ : contained in *D*.
  - Define

$$H(y) = \int_0^1 y^\top g(ty) \mathrm{d}t.$$

• Differentiation with respect to  $y_k$ , and symmetry assumption:

$$\frac{\partial g_i}{\partial y_k} = \frac{\partial g_k}{\partial y_i}$$

 $\bullet \Rightarrow$ 

•  $\Rightarrow$ 

$$\begin{aligned} \frac{\partial H}{\partial y_k} &= \int_0^1 (g_k(ty) + y^\top \frac{\partial g}{\partial y_k}(ty)t) \mathrm{d}t \\ &= \int_0^1 \frac{\mathrm{d}}{\mathrm{d}t} (tg_k(ty)) \mathrm{d}t = g_k(y) \end{aligned}$$

 $\nabla H=g. \quad \text{ for a particular of the set of$ 

Numerical methods for ODEs

• Gradient system:

- $\frac{\mathrm{d}x}{\mathrm{d}t} = -\nabla F(x);$
- F: potential function.
- LEMMA:
  - Hamiltonian system: gradient system iff H: harmonic.

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- PROOF:
  - Suppose that H: harmonic, i.e.,

$$\frac{\partial^2 H}{\partial p^2} + \frac{\partial^2 H}{\partial q^2} = 0.$$

• Jacobian of  $J^{-1}\nabla H$ : symmetric

$$(J^{-1}\nabla H)' = \begin{pmatrix} -\frac{\partial^2 H}{\partial p \partial q} & -\frac{\partial^2 H}{\partial q^2} \\ \frac{\partial^2 H}{\partial p^2} & \frac{\partial^2 H}{\partial p \partial q} \end{pmatrix}$$

• Integrability lemma  $\Rightarrow$  there exists V s.t.  $J^{-1}\nabla H = \nabla V \Rightarrow$ Hamiltonian system: gradient system.

- Suppose that Hamiltonian system: gradient system.
- There exists V s.t.

$$\frac{\partial V}{\partial p} = \frac{\partial H}{\partial q} \quad \text{and} \quad \frac{\partial V}{\partial q} = -\frac{\partial H}{\partial p}.$$
$$\Delta H := \frac{\partial^2 H}{\partial p^2} + \frac{\partial^2 H}{\partial q^2} = 0.$$

 $\Rightarrow$ 

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- EXAMPLE:
  - Hamiltonian system with  $H(p,q) = p^2 q^2$ : gradient system.

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Numerical methods for ODEs



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