Lecture 1: Some basics

Habib Ammari

Department of Mathematics, ETH Zürich

Numerical methods for ODEs

Habib Ammari

- 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,..., dⁿx(t)/dtⁿ: its derivatives.
- φ ∈ Cⁿ(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:

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

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 $i = 1, 2, ..., n$.

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

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

- EXAMPLE:
 - Consider the second order ODE:

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

• \Rightarrow

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

《口》《聞》《臣》《臣》

• 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 $x_0 \in J$.
- $g(x_0) = 0$ 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: $y(t) = x(t)/t \Rightarrow ydy = dt/t$

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

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

・ロト ・回ト ・ヨト ・ヨト

- 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:

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

 $\bullet \Rightarrow$

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

Image: A mathematical states and a mathem

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

< ∃ →

- 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 ∈ C¹(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 ω .
- Differential equation: exact equation.

- THEOREM: Implicit function theorem
 - Suppose that F(t, x): continuously differentiable in a neighborhood of (t₀, x₀) ∈ ℝ × ℝ^d and F(t₀, x₀) = 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 − t₀| < δ} s.t.

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

- THEOREM:
 - Suppose that ω : exact form with potential F s.t.

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

F(t,x) = F(t₀, x₀) implicitly defines a function x ∈ C¹(I) for some open interval I containing t₀, 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 Ω if

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

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

- PROPOSITION:
 - Exact differential form $\omega = f dt + g dx$ with a potential $F \in C^2$: closed if

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

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

- Converse: also true if Ω : 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

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

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.

- 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,

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

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

- 4 聞 と 4 直 と 4 直 と

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

$$\begin{split} &\frac{\mathrm{d}}{\mathrm{d}t}H(p(t),q(t)) = \frac{\partial H}{\partial p}(p(t),q(t))\frac{\mathrm{d}p}{\mathrm{d}t} + \frac{\partial H}{\partial q}(p(t),q(t))\frac{\mathrm{d}q}{\mathrm{d}t} \\ &= -\frac{\partial H}{\partial p}(p(t),q(t))\frac{\partial H}{\partial q}(p(t),q(t)) + \frac{\partial H}{\partial q}(p(t),q(t))\frac{\partial H}{\partial p}(p(t),q(t)) \\ &= 0. \end{split}$$

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

-∢ ≣ →

- 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

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

- 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 $A^{\top}JA = J$.
- DEFINITION Symplectic mapping
 - Differentiable map g : U → ℝ²ⁿ: 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.

A B + A B +

• PROOF:

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

• Chain rule
$$\Rightarrow$$

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

• ⇒

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

• ⇒

・ロン ・雪 と ・ ヨ と ・ ヨ と

- 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.

A B M A B M

• PROOF:

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

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

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

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

$$= 0;$$

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

<ロ> <同> <同> < 同> < 同>

.

• $\partial \phi_t / \partial y_0$ 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) .

▲母 ▶ ▲ 国 ▶ ▲ 国 ▶

- Symplecticity of the flow: characteristic property of the Hamiltonian system.
- THEOREM:
 - $f: U \to \mathbb{R}^{2n}$: 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 ϕ_t : symplectic; prove local existence of a Hamiltonian H s.t. $f(x) = J^{-1} \nabla H(s)$.
 - $\frac{\partial \phi_t}{\partial y_0}$: 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
 - $D \subset \mathbb{R}^d$: open set; $g : D \to \mathbb{R}^d \in \mathcal{C}^1$.
 - Suppose that the Jacobian g'(y): symmetric for all $y \in D$.
 - For every y₀ ∈ D, there exists a neighborhood of y₀ 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.

- ₹ 🖬 🕨

- 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

- ∢ ≣ ▶

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

・ロト ・回ト ・ヨト ・ヨト