Lecture 1: Some basics

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Some basics

• 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.
Some basics

- 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.
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• 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.**
Some basics

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

\[
\frac{d\theta(t)}{dt} = 1 - \cos \theta(t) + (1 + \cos \theta(t))f(t);
\]

\(f(t)\): inputs to the model.

- \(\theta \in [0, 2\pi]; \theta = \pi\) the neuron spikes \(\rightarrow\) produces an action potential.

- Change of variables, \(x(t) = \tan(\theta(t)/2)\), \(\rightarrow\) 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.
Some basics

• **FitzHugh-Nagumo model:**

\[
\begin{align*}
\frac{dV}{dt} &= f(V) - W + I, \\
\frac{dW}{dt} &= a(V - bW);
\end{align*}
\]

- $f(V)$: 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.
Some basics

- **Langevin equation** of motion for a single particle:

\[
\frac{dx(t)}{dt} = -ax(t) + \eta(t);
\]

- \(x(t)\): position of the particle at time instant \(t\), \(a > 0\): coefficient of friction, and \(\eta\): 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**.
Some basics

• Vander der Pol equation:

\[ \frac{d^2x(t)}{dt^2} - a(1 - x^2(t)) \frac{dx(t)}{dt} + x(t) = 0; \]

• \( a \): positive parameter, which controls the nonlinearity and the strength of the damping.

• Generate waveforms corresponding to electrocardiogram patterns.

• Nonlinear ODE of order 2.
Some basics

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

• ODE of order $n$:

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

• $x$: real-valued unknown function and $dx(t)/dt, ..., d^n x(t)/dt^n$: its derivatives.

• $\varphi \in C^n(I)$: solution of the differential equation if $I$: open interval, for all $t \in I$,

\[ (t, \varphi(t), \frac{\partial \varphi}{\partial t}(t), ..., \frac{\partial^n \varphi}{\partial t^n}(t)) \in \Omega \]

and

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

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

• $n$-th order ODE:

\[ (\ast \ast \ast) \quad x^{(n)}(t) = f(t, x, \frac{dx}{dt}, ..., \frac{d^{n-1}x}{dt^{n-1}}), \quad t \in I. \]

• $x(t) \in \mathbb{R}^d$ 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 (\ast \ast \ast) 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 $i = 1, 2, ..., n$.

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

\[ \frac{dy}{dt} = F(t, y(t)). \]
Some basics

• EXAMPLE:
  • Consider the second order ODE:

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

  • \[\Rightarrow\]

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

- 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 basics

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

- **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
    \[
    (\ast \ast \ast \ast) \quad \frac{dx}{dt} = f(t)g(x).
    \]
  - \( t_0 \in I \) 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
    \( (\ast \ast \ast \ast) \).
  - Suppose \( g(x_0) \neq 0 \rightarrow g \neq 0 \) in a neighborhood of \( x_0 \) ⇒
    \[
    \frac{dx}{g(x)} = f(t)dt.
    \]
  - Integration ⇒
    \[
    \int \frac{dx}{g(x)} = \int f(t)dt + c;
    \]
    \( c \): constant uniquely determined by the initial condition.
Some basics

- $F$ 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.
Some basics

• **EXAMPLE:**
  
  • Consider the following ODE:
  
  \[
  \begin{align*}
  \frac{dx}{dt} &= \frac{1 + 2t}{\cos x(t)}, \\
  x(0) &= \pi.
  \end{align*}
  \]
  
  • \(g(x) = \frac{1}{\cos x}\) 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 \(x(0) = \pi \Rightarrow C = 0\).
Some basics

• Taking the arcsin ⇒ $x(t) = \arcsin(t^2 + t)$: not the solution because $x(0) = \arcsin(0) = 0$.

• $\arcsin$: inverse of sin on $[-\pi/2, \pi/2]$; $x(t)$: takes the values in a neighborhood of $\pi$.

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

• Correct solution:

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

- Change of variables:
  - Consider the following ODE:
    \[
    \frac{dx}{dt} = f\left(\frac{x(t)}{t}\right);
    \]
    \(f : I \subset \mathbb{R} \rightarrow \mathbb{R}\): 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.
Some basics

• EXAMPLE:
  • Consider
    \[ \frac{dx}{dt} = \frac{t^2 + x^2}{xt} . \]
  • \( f(s) = s + 1/s \) with \( s = x/t \).
  • Change of variable: \( y(t) = x(t)/t \Rightarrow ydy = dt/t \)
  • \( \Rightarrow \)
    \[ (1/2)y^2 = \ln t + C. \]
  • \( \Rightarrow \)
    \[ x(t) = \pm t \sqrt{2(\ln t + C)}. \]
Some basics

- **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 \(\mu(t)\).
Some basics

- $\mu(t)$ s.t.

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

- Taking derivatives $\Rightarrow$

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

- Integration $\Rightarrow$

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

up to a multiplicative constant.

- Transformed equation:

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

- $\Rightarrow$

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

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

- $\mu(t)$: integrating factor.
Some basics

- **EXAMPLE:**
  - Consider

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

- \( p(t) = 1/(t + 1) \) and \( g(t) = (1 + t)^2 \).
- **Integrating factor:**

\[
\mu(t) = \exp\left(\int_0^t p(s)ds\right) = e^{\ln(t+1)} = t + 1.
\]

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

- **Initial condition** \( x(0) = 1 \) \( \Rightarrow C = 1. \)
Some basics

- **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**.
Some basics

• Important examples of ODEs:
  • Autonomous ODEs;
  • Exact equations;
  • Hamiltonian systems.
Some basics

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

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

\[
F(y) = \begin{pmatrix} 1 \\ f(t, x(t)) \end{pmatrix}.
\]
Some basics

• **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:
    \[
    f(t, x(t)) + g(t, x(t)) \frac{dx}{dt} = 0
    \]
    satisfying the initial condition \( x(t_0) = x_0 \) for some \( (t_0, x_0) \in \Omega \).

• **Differential form:**
  \[
  \omega = f(t, x)dt + g(t, x)dx.
  \]

• **DEFINITION:** Differential form: **exact** if there exists \( F \in C^1(\Omega) \) s.t.
  \[
  \omega = dF = \frac{\partial F}{\partial t} dt + \frac{\partial F}{\partial x} dx.
  \]

• \( F \): potential of \( \omega \).
• Differential equation: **exact equation**.
Some basics

- **THEOREM**: Implicit function theorem
  - Suppose that \( F(t, x) \): continuously differentiable in a neighborhood of \((t_0, x_0) \in \mathbb{R} \times \mathbb{R}^d\) and \( F(t_0, x_0) = 0 \).
  - Suppose that \( \frac{\partial F}{\partial x}(t_0, x_0) \neq 0 \).
  - 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 \( \{|t - t_0| < \delta\} \) s.t.
    \[
    F(t, x) = 0 \iff x = x(t).
    \]
Some basics

THEOREM:

• Suppose that \( \omega: \) exact form with potential \( F \) s.t.

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

• \( F(t, x) = F(t_0, x_0) \) implicitly defines a function \( x \in C^1(I) \) for some open interval \( I \) containing \( t_0 \), which solves

\[
f(t, x(t)) + g(t, x(t))\frac{dx}{dt} = 0
\]

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

• Solution: unique on \( I \).
Some basics

- **PROOF:**
  - Suppose without loss of generality that $F(t_0, x_0) = 0$.
  - **Implicit function theorem** ⇒ 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 $F(t, x(t)) = 0$,
    $$0 = \frac{d}{dt} F(t, x(t)) = \frac{\partial F}{\partial t} (t, x(t)) + \frac{\partial F}{\partial x} (t, x(t)) \frac{dx}{dt} = f(t, x(t)) + g(t, x(t)) \frac{dx}{dt}.$$  
  - ⇒ $x(t)$: solution of the differential equation.
  - $x(t_0) = x_0$.
  - If $z \in C^1(I)$: solution s.t. $z(t_0) = x_0$, then
    $$\frac{d}{dt} F(t, z(t)) = 0 \implies F(t, z(t)) = F(t_0, z(t_0)) = 0 \implies z(t) = x(t).$$
Some basics

- **DEFINITION:**
  - \( f, g \in C^1(\Omega) \).
  - 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 \( \omega = f \, dt + g \, dx \) 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 \( \Omega \): simply connected.

- Closed forms always have a potential (at least locally).
Some basics

• \textbf{EXAMPLE:}
  
  • Consider

\[ tx^2 + x - t \frac{dx}{dt} = 0. \]

  • \( f(t, x) = tx^2 + x \) and \( g(t, x) = -t \).

  • Not exact:

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

• \textbf{EXAMPLE:}

  • Consider

\[ t + \frac{1}{x} - \frac{t}{x^2} \frac{dx}{dt} = 0 \]

  • \textbf{Exact equation with the potential function} \( F \):

\[ F(t, x) = \frac{t^2}{2} + \frac{t}{x} + C, \quad C \in \mathbb{R}. \]

  • \( F(t, x) = 0 \) implicitly defines the solutions (locally for \( t \neq 0 \) and \( x \neq 0 \) s.t. \( \partial F / \partial x(t, x) \neq 0 \)).
Some basics

- Hamiltonian systems:
  - **DEFINITION:**
    - \( M \): subset of \( \mathbb{R}^d \) and \( H : \mathbb{R}^d \times M \to \mathbb{R} : C^1 \) function.
    - Hamiltonian system with Hamiltonian \( H \): first-order system of ODEs
      
      \[
      \begin{align*}
        \frac{dp}{dt} &= -\frac{\partial H}{\partial q}(p, q), \\
        \frac{dq}{dt} &= \frac{\partial H}{\partial p}(p, q).
      \end{align*}
      \]
  - **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 \( V \), 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.
Some basics

- **Invariant** for a system of ODEs:
  - **DEFINITION:**
    - $\Omega = I \times D; \ I \subset \mathbb{R} \text{ and } D \subset \mathbb{R}^d$.
    - Consider
      $$\frac{dx}{dt} = f(t, x(t));$$
    - $f : \Omega \rightarrow \mathbb{R}^d$.
    - $F : D \rightarrow \mathbb{R}$: invariant if $F(x(t)) = \text{Constant}$.
    - $(t, x) \in I \times D$: stationary point if $f(t, x) = 0$. 

Numerical methods for ODEs

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Some basics

- Example:
  - Lotka-Volterra's ODEs:
    \[
    \begin{align*}
    \frac{du}{dt} &= u(v - 2), \\
    \frac{dv}{dt} &= v(1 - u).
    \end{align*}
    \]
  - 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.
Some basics

- Differentiation with respect to time,

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

\[
= v - 2 - \frac{du}{dt} + 2(1 - u) - \frac{dv}{dt}
\]

\[
= (v - 2) - u(v - 2) + 2(1 - u) + v(1 - u)
\]

\[
= (v - 2)(1 - u) + (2 - v)(1 - u)
\]

\[
= 0.
\]
Some basics

• **LEMMA:**
  
  • Hamiltonian $H$: invariant of the associated Hamiltonian system.

• **PROOF:**
  
  $$\frac{d}{dt} H(p(t), q(t)) = \frac{\partial H}{\partial p} (p(t), q(t)) \frac{dp}{dt} + \frac{\partial H}{\partial q} (p(t), q(t)) \frac{dq}{dt}$$

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

  $$= 0.$$ 

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

- **EXAMPLE:**
  - Consider
    \[
    \begin{align*}
    \frac{dp}{dt} &= -\sin q,
    
    \frac{dq}{dt} &= p.
    \end{align*}
    \]
  - \( H(p, q) = \frac{1}{2} p^2 - \cos q: \)
    \[
    \begin{align*}
    \frac{\partial H}{\partial q} &= \sin q = -\frac{dp}{dt}, \\
    \frac{\partial H}{\partial p} &= p = \frac{dq}{dt}.
    \end{align*}
    \]
Some basics

- **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
    \[
    \frac{dx}{dt} = J^{-1} \nabla H(x).
    \]
Some basics

- **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 $g : U \to \mathbb{R}^{2n}$: 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,

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

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

- **PROOF:**
  - \( x = (p, q)^T, \ y = g(p, q)^T; \ G(y) := H(x). \)
  - **Chain rule** \( \Rightarrow \)
  
  \[
  \frac{\partial}{\partial x} H(x) = \frac{\partial}{\partial x} G(y) = \frac{\partial}{\partial y} G(y) \frac{\partial y}{\partial x} (x)
  \]
  
  \[
  = (\nabla_y G(y))^T g'(p, q).
  \]
Some basics

\[ \frac{dy}{dt} = g'(p, q) \frac{dx}{dt} \]

\[ = g'(p, q) J^{-1} \left( \frac{\partial H(x)}{\partial x} \right)^T \]

\[ = g' J^{-1} g' \nabla_y G(y) \]

\[ = J^{-1} \nabla_y G(y). \]
Some basics

- **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 \( t = 0 \).
Some basics

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

- PROOF:
  - $y_0 = (p_0, q_0)$.
  -
    $$\frac{d}{dt} \left( \left( \frac{\partial \phi_t}{\partial y_0} \right)^\top J \left( \frac{\partial \phi_t}{\partial y_0} \right) \right)$$
    $$= \left( \frac{\partial \phi_t}{\partial y_0} \right)^\top J \left( \frac{\partial \phi_t}{\partial y_0} \right) + \left( \frac{\partial \phi_t}{\partial y_0} \right)^\top J \left( \frac{\partial \phi_t}{\partial y_0} \right)'$$
    $$= \left( \frac{\partial \phi_t}{\partial y_0} \right)^\top \nabla^2 H J^{-1} \left( \frac{\partial \phi_t}{\partial y_0} \right) + \left( \frac{\partial \phi_t}{\partial y_0} \right)^\top J J^{-1} \nabla^2 H \left( \frac{\partial \phi_t}{\partial y_0} \right)$$
    $$= 0;$$
  - $\nabla^2 H$: Hessian matrix of $H(p, q)$ (symmetric).
Some basics

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

\[
\left( \frac{\partial \phi_t}{\partial y_0} \right)^T J \left( \frac{\partial \phi_t}{\partial y_0} \right) = J
\]

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

Some basics

• **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 \( t \).
Some basics

- **PROOF:**
  - Necessity $\Leftarrow$ Poincaré’s Theorem.
  - Suppose that $\phi_t$: symplectic; prove local existence of a Hamiltonian $H$ s.t. $f(x) = J^{-1} \nabla H(s)$.
  - $\frac{\partial \phi_t}{\partial y_0}$: solution of
    \[
    \frac{dy}{dt} = f'(\phi_t(y_0))y;
    \]
  - $\Rightarrow$
    \[
    \frac{d}{dt} \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 \left[ f'(\phi_t(y_0))^\top J + Jf' \right] \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 $H$. 

Numerical methods for ODEs Habib Ammari
Some basics

• **LEMMA:** Integrability lemma
  
  • $D \subset \mathbb{R}^d$: open set; $g: D \to \mathbb{R}^d \in C^1$.
  • Suppose that the Jacobian $g'(y)$: symmetric for all $y \in D$.
  • For every $y_0 \in D$, there exists a neighborhood of $y_0$ and a function $H(y)$ s.t.
    
    $$g(y) = \nabla H(y)$$

  on this neighborhood.
Some basics

• **PROOF:**
  • Suppose that \( y_0 = 0 \), and consider a ball around \( y_0 \): contained in \( D \).
  • Define
    \[
    H(y) = \int_0^1 y^\top g(ty)dt.
    \]
  • Differentiation with respect to \( y_k \), and symmetry assumption:
    \[
    \frac{\partial g_i}{\partial y_k} = \frac{\partial g_k}{\partial y_i}
    \]
  • \( \Rightarrow \)
    \[
    \frac{\partial H}{\partial y_k} = \int_0^1 (g_k(ty) + y^\top \frac{\partial g}{\partial y_k}(ty)t)dt
    = \int_0^1 \frac{d}{dt}(tg_k(ty))dt = g_k(y)
    \]
  • \( \Rightarrow \)
    \[
    \nabla H = g.
    \]
Some basics

- Gradient system:
  \[
  \frac{dx}{dt} = -\nabla F(x);
  \]
  - $F$: potential function.

- **LEMMA:**
  - Hamiltonian system: gradient system iff $H$: harmonic.
Some basics

• 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.
Some basics

• Suppose that Hamiltonian system: gradient system.

• There exists $V$ s.t.

$$\frac{\partial V}{\partial p} = \frac{\partial H}{\partial q} \quad \text{and} \quad \frac{\partial V}{\partial q} = -\frac{\partial H}{\partial p}.$$ 

• $\Rightarrow$

$$\Delta H := \frac{\partial^2 H}{\partial p^2} + \frac{\partial^2 H}{\partial q^2} = 0.$$
Some basics

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