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:
    \[ C \frac{dx(t)}{dt} + gx(t) = f(t), \]
    where:
    - \(x(t)\): 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 → produces an action potential.

- Change of variables, \(x(t) = \tan(\theta(t)/2)\), → quadratic model

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

- Population growth under competition for resources:

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

\(r\) and \(k\): positive parameters; \(x(t)\): number of cells at time instant \(t\),

\(rx(t)\): growth rate and \(-(r/k)x(t)^2\): death rate.

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

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**Numerical methods for ODEs**

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Some basics

- **FitzHugh-Nagumo model:**

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

- \(V\): 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.**
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:

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

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

• (*** ) 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
    \[
    (***) \quad \frac{dx}{dt} = f(t)g(x).
    \]
  - $t_0 \in I$ 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 $g(x_0) \neq 0 \rightarrow g \neq 0$ 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.
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.
- $(\ast \ast \ast \ast)$: separable equation.
Some basics

• EXAMPLE:
  • Consider the following ODE:
    \[
    \begin{align*}
    \frac{dx}{dt} &= \frac{1 + 2t}{\cos x(t)}, \\
    x(0) &= \pi.
    \end{align*}
    \]
  • \( g(x) = 1/\cos x \) 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:
    \[
    \frac{dx}{dt} = f\left(\frac{x(t)}{t}\right); \\
    f : I \subset \mathbb{R} \rightarrow \mathbb{R}: \text{ continuous function on some open interval } I \subset \mathbb{R}.
    \]
  • change of variable \( x(t) = ty(t); \ y(t): \text{ new unknown function}, \)
    \[
    \frac{dx}{dt} = y(t) + t \frac{dy}{dt} = f(y(t)),
    \]
  • 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:**
    \[
    \mu(t) = \exp\left(\int_0^t p(s)ds\right) = e^{\ln(t+1)} = t+1.
    \]
  
  - \(\Rightarrow \)
    \[
    x(t) = \frac{1}{t+1} \int_0^t (s + 1)^3ds + \frac{C}{t+1} = \frac{(t + 1)^3}{4} + \frac{C - \frac{1}{4}}{t+1}.
    \]
  
  - Initial condition \(x(0) = 1 \Rightarrow C = 1\).
Some basics

- **EXAMPLE:** (Bernoulli’s equation)

- Consider

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

- \( \alpha \not\in \{0, 1\} \).

- Change of variable: \( x = z^{1-\alpha} \),

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

- 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 \( f \) independent of \( t \).
  - Any ODE can be rewritten as an autonomous ODE on a higher-dimensional space.
  - \( y = (t, x(t)) \) → autonomous ODE

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

\[
F(y) = \left( \frac{1}{f(t, x(t))} \right) .
\]
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** $\Rightarrow$ 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 $F(t, x(t)) = 0$,
    
    $0 = \frac{d}{dt} F(t, x(t)) = \frac{\partial F}{\partial t} (t, x(t)) + \frac{\partial F}{\partial x} (t, x(t)) \frac{dx}{dt} = \frac{\partial F}{\partial t} (t_0, x(t_0)) + \frac{\partial F}{\partial x} (t_0, x(t_0)) \frac{dx}{dt} = f(t, x(t)) + g(t, x(t)) \frac{dx}{dt}$.

  - $\Rightarrow x(t)$: 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
    
    $\frac{d}{dt} F(t, z(t)) = 0 \iff F(t, z(t)) = F(t_0, z(t_0)) = 0 \iff z(t) = x(t)$.  

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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** 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).
Some basics

- **EXAMPLE:**
  - Consider
    \[ tx^2 + x - t \frac{dx}{dt} = 0. \]
  - \( f(t, x) = tx^2 + x \) and \( g(t, x) = -t \).
  - Not exact:
    \[ \frac{\partial f}{\partial x} = 2xt + 1 \neq \frac{\partial g}{\partial t} = -1. \]

- **EXAMPLE:**
  - Consider
    \[ t + \frac{1}{x} - t \frac{dx}{x^2 \, dt} = 0 \]
  - 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
      \[
      H(p, q) = \frac{1}{2} p^2 \frac{1}{m} + \frac{1}{2} kq^2;
      \]
      $m$ and $k$: positive constants.
    - Given a potential $V$, widely used Hamiltonian systems in molecular dynamics:
      \[
      H(p, q) = \frac{1}{2} p^\top M^{-1} p + V(q);
      \]
      $M$: symmetric positive definite matrix and $\top$: transpose.
Some basics

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

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

• Notation $\nabla H(x) := \left( \frac{\partial H}{\partial x} \right)^T = \left( \frac{\partial H}{\partial x_1}, \ldots, \frac{\partial H}{\partial x_d} \right)^T$.

• For a vector function $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$, $f(x) = (f_1(x), \ldots, f_d(x))$, we define the Jacobian matrix $f'$ of $f$ by

$$f'(x) := \begin{pmatrix}
\frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_d} \\
\vdots & \ddots & \vdots \\
\frac{\partial f_d}{\partial x_1} & \cdots & \frac{\partial f_d}{\partial x_d}
\end{pmatrix}.$$
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 $A^TJA = J$. 

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• DEFINITION Symplectic mapping
  • Differentiable map \( g : U \rightarrow \mathbb{R}^{2n} \): symplectic if the Jacobian matrix \( g'(p, q) \): everywhere symplectic, i.e., if

  \[
  g'(p, q)^\top J g'(p, q) = J.
  \]

  • 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:**
  
  • \( x = (p, q)^\top, \ y = g(p, q)^\top; \ G(y) := H(x). \)
  • **Chain rule \( \Rightarrow \)**

\[
\frac{\partial}{\partial x} H(x) = \frac{\partial}{\partial x} G(y) = \frac{\partial}{\partial y} G(y) \frac{\partial y}{\partial x}(x)
\]

\[
= (\nabla_y G(y))^\top g'(p, q).
\]
Some basics

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

\[ = g'(p, q) J^{-1} \left( \frac{\partial H(x)}{\partial x} \right)^\top \]

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

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

- **DEFINITION:**
  - Flow:
    \[
    \phi_t(p_0, q_0) = (p(t, p_0, q_0), q(t, p_0, q_0));
    \]
  - \(\phi_t : U \rightarrow \mathbb{R}^{2d}, U \subset \mathbb{R}^{2d};\)
  - \(p_0\) 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:**
  
  • \( y_0 = (p_0, q_0) \).
  
  \[
  \frac{d}{dt} \left( \left( \frac{\partial \phi_t}{\partial y_0} \right)^T J \left( \frac{\partial \phi_t}{\partial y_0} \right) \right) = \left( \frac{\partial \phi_t}{\partial y_0} \right)^T J \left( \frac{\partial \phi_t}{\partial y_0} \right) + \left( \frac{\partial \phi_t}{\partial y_0} \right)^T J \left( \frac{\partial \phi_t}{\partial y_0} \right)' \]
  
  \[
  = \left( \frac{\partial \phi_t}{\partial y_0} \right)^T \nabla^2 H J^{-T} J \left( \frac{\partial \phi_t}{\partial y_0} \right) + \left( \frac{\partial \phi_t}{\partial y_0} \right)^T JJ^{-1} \nabla^2 H \left( \frac{\partial \phi_t}{\partial y_0} \right) \]
  
  \[
  = 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 $(p_0, q_0)$. 

Numerical methods for ODEs

Habib Ammari
Some basics

• **Symplecticity** of the flow: characteristic property of the Hamiltonian system.

• **THEOREM:**
  - \( f : U \rightarrow \mathbb{R}^{2n} \): 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 \( \iff \) 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 \( H \).
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.