Lecture 3 :

Dynamical systems governed by ordinary differential equations

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October - December 2010

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Typical implementation :

- Hamiltonian dynamics, spatially uniform systems at the macroscopic level of description.
- Evolution in the form of ODE's

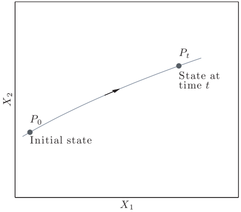
$$\frac{dX_i}{dt} = F_i\left(X_1, ...X_n, \lambda\right)$$

λ accounts for such parameters as rate constants (chemistry), birth rates (biology). etc ...

Typically, no analytic solutions available in presence of nonlinearities.

Qualitative analysis
Geometric view

Phase space



Phase space trajectory

- Uniqueness theorem. Forbids intersection of trajectories.

Invariant sets

Sets in phase space that are mapped onto themselves by the evolution laws. Simplest case :

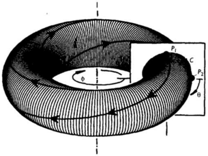
- **O-d sets** : fixed points, solution of $F_i\left(X_1, ...X_n, \lambda\right) = 0$ representing physically the steady states of the system at hand
- **1-d sets** : closed curves, representing periodic behavior.

Qualitative analysis

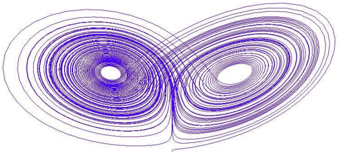
Geometric view

High dimensional invariant sets

- Tori (quasi periodic behavior),

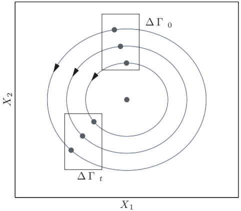


- Fractals (chaotic behavior).



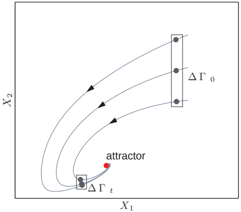
Qualitative analysis
Geometric view

Conservative and dissipative systems, attractors.



Phase space trajectory

- Conservative system : $|\Delta\Gamma_0| = |\Delta\Gamma_t|$. (typical signature of Hamiltonian dynamics)



- Dissipative system : $|\Delta\Gamma_t| < |\Delta\Gamma_0|$. (for sufficiently long times)

Qualitative analysis
Stability

Response to a perturbation removing the system from an initial "reference" set s

$$X_i\,(t) = X_{i,s} + \delta x_i\,(t)$$

- Stability : system remains in a neighborhood of $X_{i,s}$
- Assymptotic stability : $\delta x_i\,(t) \to 0$ as $t \to \infty$

Self-organization viewed as a problem of loss of stability of the "trivial" states (e.g., the fixed points) and evolution towards more intricate attractors.

Linear stability analysis

$$\frac{dX_i}{dt} = F_i\left(\{X_j\}, \lambda\right) \qquad j = 1, \ldots n$$

- Search for reference state, usually among the steady states

$$F_i\left(\{X_{j,s}\}, \lambda\right) = 0$$

- Linearize around $\{X_{j,s}\}$

$$X_j = X_{j,s} + \delta x_j \qquad \frac{d\delta x_i}{dt} = \sum_j \left(\frac{\partial F_i}{\partial X_j}\right)_s \delta x_j$$

Solution in the form
$\delta x_i = u_i \mathrm{e}^{\omega_\alpha t}$

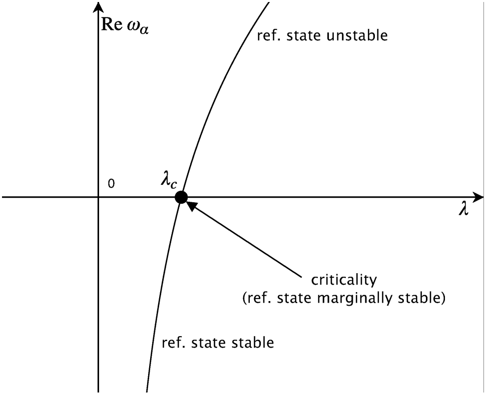
- Determine the eigenvalues ω_α $(\alpha = 1, \ldots n)$ of the operator (Jacobian matrix)

$$\underset{\approx}{J} = \left(\frac{\partial F_i}{\partial X_j}\right)_s$$

as roots of the characteristic equation $\det \left| \left(\frac{\partial F_i}{\partial X_j}\right)_s - \omega \delta_{ij}^{\mathsf{kr}} \right| = 0$

Qualitative analysis
Linear stability analysis

In particular, parameter values λ_c at which the real part of one of the ω_α's changes sign :
$\mathrm{Re}\ \omega_\alpha\ (\lambda_c) = 0$



Perturbation analysis
Bifurcation analysis

Bifurcation analysis

Parameter λ_c beyond which the steady state X_{is} becomes unstable :

- Perturbation δx will start to grow. Linearization around X_{is} will no longer be valid beyond some stage.
- Take into account nonlinear terms in the equations $\Rightarrow$ growth of the perturbation saturating, leading to a new solution ?

Explore the vicinity of λ_c by seeking for new solutions **bifurcating** from the reference state.

$$\frac{d\delta x_i}{dt} = \sum_j J_{ij}\delta x_j + \underbrace{\mathrm{NL}\,(\delta x_1, \ldots \delta x_n)}_{\text{nonlinear part}}$$

expand δx in powers of a smallness parameter.

$$\delta x_j = \epsilon \delta x_j^{(1)} + \epsilon^2 \delta x_j^{(2)} + \cdots$$

where ϵ ($|\epsilon| << 1$) is related to the distance from criticality, $\lambda - \lambda_c$

Asymptotic analysis

Explore limiting cases where some parameters (usually parameter ratios) $\rightarrow \infty$ and variables switch from small to large values in phase space.

Application : Elimination of fast variables

Multivariate systems (tens or hundreds of variables in typical situation).
Reduction to a low-order dynamics in presence of widely separated time scales due to order of magnitude differences in the values of parameters and/or state variables.

Some typical examples

- Catalytic reactions :

$$\underbrace{E}_{\text{enzyme}} + \underbrace{S}_{\text{substrate}} \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} \underbrace{C}_{\text{complex}} \xrightarrow{k} E + \underbrace{P}_{\text{product}} \qquad \begin{array}{l} [C],\ [E] << S \\ k >> k_1,\ k_{-1} \end{array}$$

- Combustion :

$$E >> kT$$

$\rightarrow$ reactions proceed more slowly than does energy transport

Application : Elimination of fast variables

Cast original equations, upon performing an appropriate change of variables and parameters, in the form

$$\begin{aligned} \frac{dX}{dt} &= F(X, Y, \epsilon) \quad \text{(slow variables)} \\ \epsilon \frac{dY}{dt} &= G(X, Y, \epsilon) \quad \text{(fast variables)} \quad (\epsilon << 1) \end{aligned}$$

Tikhonov theorem

Under appropriate conditions (G invertible) the limit $\epsilon \to 0$ can be taken and Y variables can be eliminated :

$$\begin{aligned} & G(X, Y, 0) = 0 \\ \Rightarrow \quad & Y = W(X) \quad \text{("slow manifold" eq.)} \\ \Rightarrow \quad & \frac{dX}{dt} = F(X, W(X)) = f(X) \end{aligned}$$

Notice that elimination of fast variables reduces the dimensionality of phase space. In this sense the dynamics of fast variables constitues a **singular perturbation** of the slow variables.

Application : Elimination of fast variables
Michaelis-Menten kinetic

Case study I : Michaelis-Menten kinetics

$$\underbrace{E}_{\text{enzyme}} + \underbrace{S}_{\text{substrate}} \underset{k_{-1}}{\overset{k_1}{\rightleftarrows}} \underbrace{C}_{\text{complex}} \xrightarrow{k} E + \underbrace{P}_{\text{product}}$$

The evolution equations are

$$\begin{aligned} \frac{dS}{dt} &= -k_1 ES + k_{-1} C \\ \frac{dE}{dt} &= -\frac{dC}{dt} = -k_1 ES + (k_{-1} + k) C \end{aligned}$$

with $E + C = Cst = E_0$

Quasi steady-state assumption for C :

$$\frac{1}{k_{-1} + k} \frac{dC}{dt} = \frac{k_1}{k_{-1} + k} ES - C$$

k large, $k_1 S/k$ finite, amount of $S >> E$ or C

Application : Elimination of fast variables
Michaelis-Menten kinetic

Left hand side multiplied by $\epsilon \approx k^{-1} << 1$. We take the limit $\epsilon \to 0$ (Tikhonov's theorem). Thus

$$C \approx \frac{k_1}{k_{-1}+k} ES \qquad or,$$

$$\begin{aligned} C &\approx \frac{k_1}{k_{-1}+k}\left(E_0 - C\right)S \\ C &\approx \frac{E_0 S}{\frac{k_{-1}+k}{k_1} + S} = \frac{E_0 S}{K+S} \end{aligned}$$

where K is the **Michaelis-Menten constant.**
Substituting into original equations :

$$\frac{dS}{dt} = -k_1 ES + k_{-1}C \approx kC$$

or

$$\frac{dS}{dt} = -\frac{kE_0 S}{K+S}$$

Application : Elimination of fast variables
Derivation of the Hill function

Case study II : Derivation of the Hill function

Hill kinetics arises when E possesses multiple fixation sites such that, e.g.,

$$E + 2S \leftrightarrows C \rightarrow \ldots$$

A more elaborate way would be to decompose into steps,

$$\begin{aligned} E + S &\leftrightarrows C_1 \\ C_1 + S &\leftrightarrows C_2 \\ &\ldots \end{aligned}$$