Simulation, Analysis, and Validation of Computational Models

— 4. Nonlinear Systems—

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Overview

- Non-linear systems
- Bifurcations
- Chaos
- Numerical integration

Recap: Linear systems

- Equation $\dot{x} = Ax$
- Including constant terms:
  - Standard form $\dot{x} = Ax - b$, i.e. b always affects $\dot{x}$
  - Easier form $\dot{x} = A\left(x - \tilde{b}\right)$ with $\tilde{b} = A^{-1}b$, if A^{-1} exists, otherwise some components of $\tilde{b}$ may not affect $\dot{x}$
- Behaviour depends on the eigenvalues of A
  - negative real part: stable
  - positive real part: unstable
  - non-zero imaginary part: rotational behaviour
- Often useful for short-term prediction or modelling

Last time: General ODE case

Characterise the system dynamics by an arbitrary function f

$$\frac{dx(t)}{dt} = f(x(t)) \qquad (1)$$

Expand f into a Taylor series (may not always be a good approximation)

$$f(x) = f(x_0) + \frac{df(x_0)}{dx}(x - x_0) + \frac{1}{2}\frac{d^2 f(x_0)}{dx^2}(x - x_0)^2 + \frac{1}{6}\frac{d^3 f(x_0)}{dx^3}(x - x_0)^3 + \dots$$

Often we can consider linear terms only (and constant terms) as a linearisation of the form (1)

$$\frac{dx(t)}{dt} = f(x_0) + \frac{df(x_0)}{dx}(x - x_0)$$

This is also how we get the dynamical matrix, i.e. $b_{ij} = \frac{df_i(x_0)}{dx_j}$, for the multidimensional linear case.

What if $\frac{df(x_0)}{dx} \approx 0$ (much smaller than higher-order terms)?

Symmetry

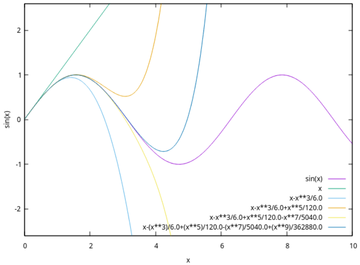
Example: Sine function (see pendulum of last lecture) is an *anti-symmetric* (or *odd*) function. Thus, the Taylor expansion (at $x_0 = 0$)

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} - \cdots + \cdots$$

contains only odd terms, due to its derivatives (check!)

$$\left.\frac{d^k \sin(x)}{dx^k}\right|_{x=0} = \begin{cases} \pm 1 & \text{for } k \text{ odd} \\ 0 & \text{for } k \text{ even} \end{cases}$$

which may reflect the symmetry of the system.



The approximation is not very good in general, but good enough near $x_0 = 0$.

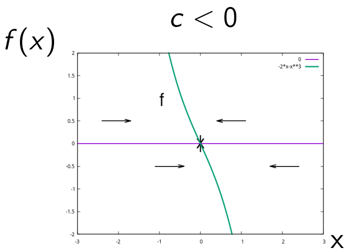
Example: Nonlinear system

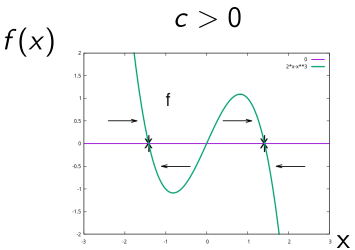
Last time, we have used $\sin x \approx x$ (for $x \approx 0$), now we consider one more term in the Taylor series of an odd function:

$$\dot{x} = f(x) = c\,x - d\,x^3 \tag{2}$$

First, remember the linear case $\dot{x} = f(x) = cx$: For $c < 0$ stable, and for $c > 0$ unstable.

The parameter d is fixed (e.g. $1/6$ for $f(x) = \sin(x)$ or here simply $d = 1$), i.e. if $c < 0$, then the cubic term (which acts in a similar way) doesn't make a difference (left), but what happens for $c > 0$?



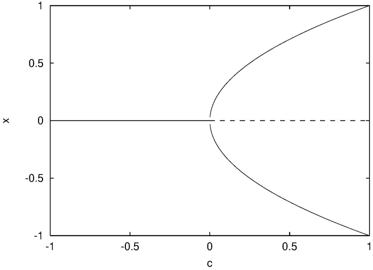


Bifurcation diagram

Fixed points occur when the dynamics comes to a halt at some $x = x^*$, i.e. $\dot{x} = f(x) = 0$.

How does the parameter c influence the fixed points?

$$\begin{aligned} \dot{x} &= f(x) \\ &= cx + x^3 \stackrel{!}{=} 0 \\ c < 0 &\rightarrow \text{one real solution} \\ x^* &= 0 \text{ (stable)} \\ c > 0 &\rightarrow \text{three real solutions} \\ x^* &= \pm\sqrt{c} \text{ or } x^* = 0 \\ & \text{(two stable, one unstable)} \end{aligned}$$



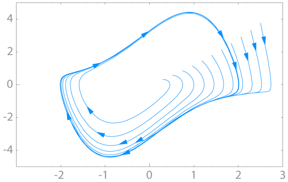
x^* depends here on c

Attractors: What can happen (apart from fixed points)?

- In linear systems we can usually describe the full dynamics: exponential growth or decay, oscillations, or combinations.
- In non-linear systems this is often not possible, and we often consider *attractors*, i.e. asymptotic states or sets of states, such as
  - fixed points (locally similar to a *node* in a linear system)
  - limit cycles (related *to a center* in a linear system, but with attraction towards the cycle), only for state space dimension ≥ 2, and combinations of limit cycles (*tori*), only for state space dimension ≥ 3
  - chaotic attractors (System does not come to a rest, but remains in a certain part of the state space), only for state space dimension ≥ 3
- Attractors are generally reached for $t \to \infty$, and if they are reached for $t \to -\infty$, we call them *unstable attractors.*
- Not included: Sets that are neither stable nor unstable (e.g. *center*)

Limit cycles

Limit cycle is a closed trajectory in state space which is approached by other trajectories that are spiralling towards it (or away from it for an unstable limit cycle).



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Van der Pol oscillator

Vibration, certain waves, neural activity is described as limit cycles

Respiration or heartbeat are controlled by complex limit cycles

Useful also in modelling and control of walking movements

Hilbert's 16(b)th problem: Find an upper bound for the number of limit cycles in 2D dynamical systems with nonlinearity of degree n (unsolved for $n > 1$).

Limit cycles: Poincaré–Andronov–Hopf bifurcation

Consider linear system (“center”)

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \end{pmatrix} = M \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

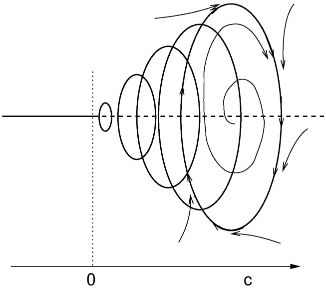
Eigenvalues of M: $\lambda_{1/2} = \pm i \Rightarrow$ solutions are $x(t) = |x_0| \begin{pmatrix} \cos(\pm t) \\ \sin(\pm t) \end{pmatrix}$

Combine with the cubic system (2):

$$\begin{aligned} \dot{y}_1 &= (c\rho - \rho^3) y_1 - y_2 \\ \dot{y}_2 &= y_1 + (c\rho - \rho^3) y_2 \\ \rho &= \sqrt[+]{y_1^2 + y_2^2} > 0 \end{aligned}$$

$c < 0$: fixed point

$c > 0$ limit cycle



Routes to chaos

Chaos refers to the behaviour of dynamical system with a sensitive dependence on initial conditions.

- Limit cycle folds over as parameters change: Period doubling
- Similarly: "baker" transformation (or cat map)
- Practically, combinations of three limit cycles often turn into chaos

Chaos is different form noise by short-term predictability. However, high-dimensional chaos is practically indistinguishable from noise.

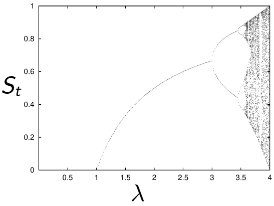
While all other slides are about continuous systems, this one is about a map (discrete time system).

Logistic map has cascade of period doublings turning into chaos

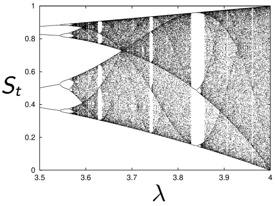
$$S_{t+1} = \lambda S_t \left(1 - S_t\right), \ \lambda \in [0,4], \ S_t \in [0,1], \ t \in \mathbb{N}$$

Fixed point: $S = \lambda S \left(1 - S\right) \Rightarrow S^* = 1 - \frac{1}{\lambda}$

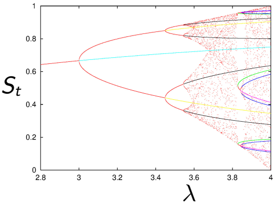
For $\lambda = 3$ this fixed point becomes unstable, and a stable two-step limit cycle appears, which becomes unstable near $\lambda = 3.45$, then a stable four-step limit cycle appears etc. This cascade converges at $\lambda \approx 3.56995$ when the dynamics becomes chaotic, albeit interspersed with periodic windows.



Relevant parameter space



close-up of chaotic region



incl. some unstable f.p.

Chaos: Toy examples

Often studied examples are 3D systems of nonlinear differential equations, such as the Roessler system

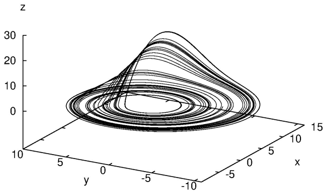
$$\dot{x} = -y - z$$
$$\dot{y} = x + ay$$
$$\dot{z} = b + z\,(x - c)$$

$a = b = 0.2, c = 5.7$

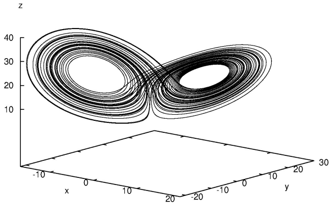
or the Lorenz system

$$\dot{x} = \sigma\,(y - x)$$
$$\dot{y} = x\,(\rho - z) - y$$
$$\dot{z} = x\,y - \beta z$$

Typical values for the constants: $\sigma = 10$, $\beta = 8/3$ and $\rho = 28$



Roessler attractor



Lorenz attractor

Chaos: Real-world examples

- The solar system seems to be a "clock work", i.e. a limit cycle. However, it's (currently very mildly) chaotic[1].
- Good drummers can produce a certain beat very precisely (limit cycle), while professional drummers may embellish the rhythm by tiny modulations (chaotic attractor).
- Similar modulation of limit cycles can occur in walking.
- Recurrent neural networks: Hopfield model can have only limit cycles. For more general models, already three interconnected neurons can produce chaotic signals.
- Controlling the blade in front of a bulldozer in heterogeneous environments may require a chaotic control strategy.
- Strategies for search and exploration may become more efficient, if autocorrelation varies. This can be achieved by chaotic (rather than noisy) driving.

[1] Malhotra R, Holman M, Ito T. (2001) Chaos and stability of the solar system. *PNAS* **98**, 12342-3.

Conclusion on Nonlinear systems

- Non-linear dynamics is predominant in all aspects nature, in society, and in complex technical systems.
- A major challenge in many fields of application of the theory is the identification of imminent qualitative changes ("tipping points").
- While linear systems are well understood, many problem in non-linear dynamics remain to be solved, to be formulated or to be discovered.
- Numerical simulation of non-linear systems are still improvable.

Numerical integration

- Goal: As there is usually no analytical solution, we need to find a numerical solution $\hat{x}(t)$ for $t \geq t_0$ for an ordinary differential equation $\dot{x} = f(x)$, given $x(t_0) = \hat{x}_0(0) = x_0$
- An algorithm that calculates $\hat{x}$ can be evaluated by the integral

$$\int_{t_0}^{t_1} (x(t) - \hat{x}(t))^2 \, dt$$

  or by the maximum of the difference $|x - \hat{x}(t)|$ or by the order of a polynomial that can still perfectly be integrated.
- Find $\dot{x}$ at several points across the interval Δt using the ODE and Taylor expansion. Weight and combine resulting values and to get an estimate for $t + \Delta t$. Add corrector for further improvement.
- Integration formulas depend on the specific method and differ in number and weights and order of points along time axis.

Numerical integration

Euler method (integrates linear functions perfectly, it's something)

$$x(t + \Delta t) = x(t) + \dot{x}(t)\,\Delta t \text{ where } \dot{x}(t) = f(x(t))$$

is simple and can be sufficient for small Δt, but it's only of order 1 so that errors can be large especially for exponential dynamics.

Example: $\dot{x}(t) = x(t)$ starting at $x(0) = 1$ using $\Delta t = 1$

$x(1) = x(0) + x(0) \cdot 1 = 2$

$x(2) = x(1) + x(1) \cdot 1 = 2 + 2 \cdot 1 = 4$

$x(3) = x(2) + x(2) \cdot 1 = 4 + 4 \cdot 1 = 8 \Rightarrow x(n) = 2^n$

At $n = 4$ Euler: 16, exp(4) =54.60: abs. error of 38.60

$\Delta t = 1$ is generally too large, but reducing step width to 0.1 still gives an abs. error of 9.34

Many better methods available.

Numerical integration: Predictor–corrector method

Combinations of any methods are possible, but for simplicity we start again with the Euler method for the Predictor step:

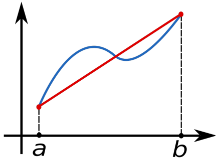
$$\tilde{x}(t+\Delta t) = x(t) + \dot{x}(t)\,\Delta t$$

Corrector step to interpolate the initial attempt with new result from the predictor using the differential equation $\dot{\tilde{x}} = f(\tilde{x}(t+\Delta t))$

$$\hat{x}(t+\Delta t) = x(t) + \frac{1}{2}\Delta t\,(\dot{x}(t) + f(\tilde{x}(t+\Delta t)))$$

which is called trapezoidal rule.

Above example: $\tilde{x}(1) = 2,\ f(\tilde{x}) = 2 \Rightarrow$
$\hat{x}(1) = 1 + \frac{1}{2}\cdot 1 \cdot (1+2) = 2.5\ (\Delta t = 1)$
(compare to $e = 2.71828$).



Numerical integration

- Explicit methods determine the state for a later time from the state of the system at present
- Implicit methods determine the solution by solving an equation involving the current state of the system and later ones.
- Direct methods: Use intermediate values to cacluate the next step
- Multi-step method: Calcluate new values based on several previous values (how to get started?)

Numerical integration: Explicit methods

- E.g. RK4 (4th order Runge-Kutta method, explicit)

$$x\left(t+\Delta t\right)=x\left(t\right)+\frac{\Delta t}{6}\left(\underbrace{k_1+2k_2+2k_3+k_4}_{\text{mixture of derivatives}}\right),$$

$$k_1=f(x\left(t\right)),$$

$$k_2=f\left(x\left(t+\frac{\Delta t}{2}\right)+\Delta t\frac{k_1}{2}\right),$$

$$k_3=f\left(x\left(t+\frac{\Delta t}{2}\right)+\Delta t\frac{k_2}{2}\right),$$

$$k_4=f\left(x\left(t+\Delta t\right)+\Delta t\, k_3\right).$$

- Solves ODEs with polynomial f of order not greater than 4 precisely.

Numerical integration: Implicit methods

- For highly non-linear ODEs, implicit methods may work better, i.e. moving forwards and backwards in time (like predictor corrector). Example: Adams-Moulton method.

$$
\begin{aligned}
x(t+\Delta t) = x(t) + \frac{h}{720} \; & (251 f(x(t+\Delta t)) + 646 f(x(t)) \\
& -264 f(x(t-\Delta t)) + 106 f(x(t-2\Delta t)) \\
& -19 f(x(t-3\Delta t)))
\end{aligned}
$$

- Need to get started (multi-step method), by calculating the first steps by more simple methods
- Solves ODEs with polynomial f of order not greater than 5 precisely.

Numerical integration: Points to remember

- Because analytical solutions are mostly unavailable, numerical integration is generally used, but can go wrong.
- Simply reducing step widths can give an idea that the system is problematic, but may be inefficient for solution
  - Complex integration methods can help and are generally used in numeric
  - Adaptive methods, step width control (not discussed here)
- Practically, 4th order Runge Kutta (RK4) is often sufficient.
- For complex or chaotic systems, implicit methods should be considered.

Next topics

- Relation between discrete and non-linear systems
- More non-linear phenomena: Collisions
- Noise
- Simulations