

Simulation and modeling of natural processes

Week 3: Dynamical systems and numerical integration

Orestis Malaspinas

General introduction to dynamical systems

What is a dynamical system?

- A system that varies through time.
- The system is described by its state $s(t)$.
- The state s can be multivariate (a vector)

$$s(t) = (s_1(t), \dots, s_n(t))^T.$$

- Examples: pendulum, population evolution, ...

Different classes of descriptions

- **Discrete** dynamical systems are described by *recurrence relations*

$$s(t + \Delta t) = f(s(t)),$$

where f is a function and Δt the time increment.

- **Continuous** dynamical systems are described by *differential equations*

$$\dot{s} \equiv \frac{ds}{dt} = f(s(t)).$$

Generality of the description: continuous case

What happens if we have second derivatives?

$$\dot{s} + \ddot{s} = f(s)$$

Let us then define

$$\begin{aligned}\dot{s} &= y, \\ \dot{y} &= f(s) - y.\end{aligned}$$

By defining $\mathbf{u}(t) \equiv (s(t), y(t))$ we have a system of the form

$$\dot{\mathbf{u}} = \mathbf{g}(\mathbf{u}).$$

Generality of the description: discrete case

“Second derivatives” equivalent to presence of a $t - \Delta t$ term

$$s(t + \Delta t) = f(s(t)) + s(t - \Delta t).$$

Similarly to continuous case

$$y(t + \Delta t) = s(t),$$

$$s(t + \Delta t) = f(s(t)) + y(t),$$

and by defining $\mathbf{u}(t) \equiv (s(t), y(t))$ we have a system of the form

$$\mathbf{u}(t + \Delta t) = g(\mathbf{u}(t)).$$

Generality of the description: continuous case

What happens if f explicitly depends on t ?

$$\dot{s} = f(s, t)$$

Let us then define

$$\dot{s} = f(s, y)$$

$$\dot{y} = 1,$$

with $y(0) = 0$. By defining $\mathbf{u}(t) \equiv (s(t), y(t))$ we have a system of the form

$$\dot{\mathbf{u}} = g(\mathbf{u}).$$

End of module

General introduction to dynamical
systems

Coming next

The random walk

The random walk

The random walk

Time evolution of particles, drunk people, ...

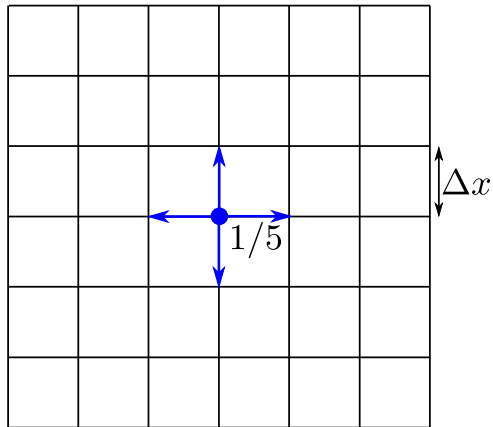
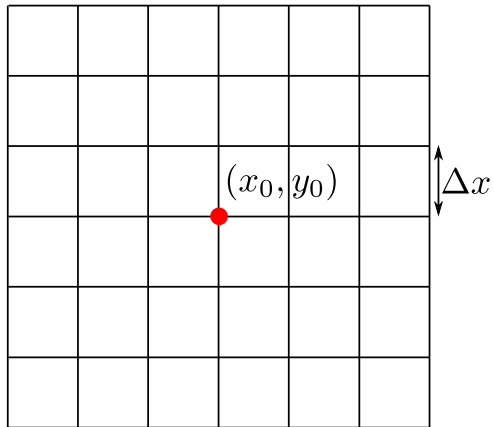
$$\begin{aligned}x(t + \Delta t) &= x(t) + \Delta t \cdot v_x(t), \\y(t + \Delta t) &= y(t) + \Delta t \cdot v_y(t),\end{aligned}$$

where (v_x, v_y) is chosen randomly in the ensemble

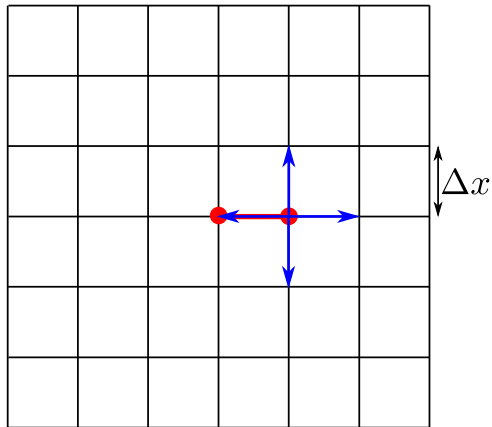
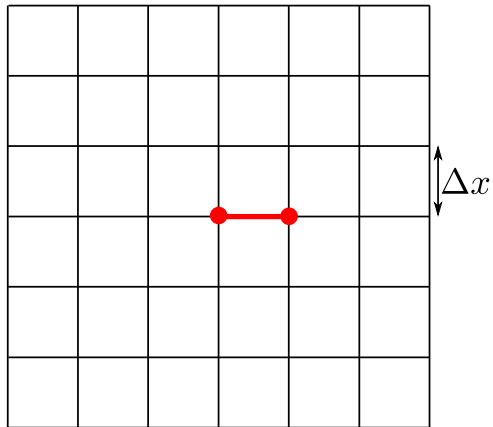
$$\{(\Delta x / \Delta t, 0), (-\Delta x / \Delta t, 0), (0, 0), (0, \Delta y / \Delta t), (0, -\Delta y / \Delta t)\},$$

where Δx and Δy are the length of the displacements in direction x and y .

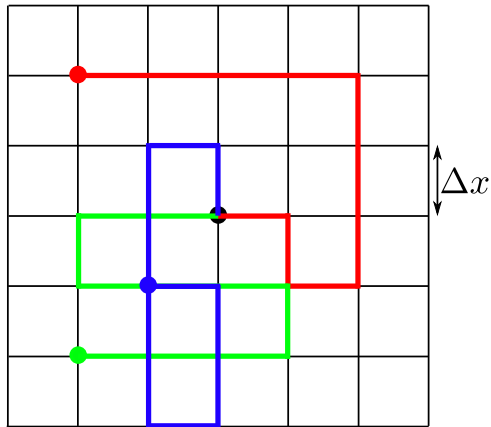
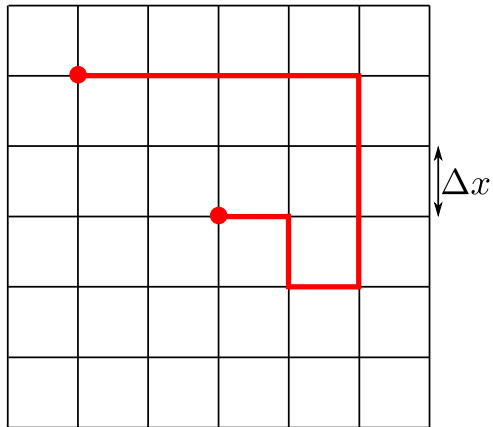
The random walk: illustration



The random walk: illustration



The random walk: illustration



The random walk: mathematical analysis

What is the “average” behavior of many random walkers?

- Initial position of the walker is $(x(0), y(0)) = (x_0, y_0)$.
- After a time $t = N \cdot \Delta t$ the position of a random walker is

$$\begin{aligned}x(t) &= x(t - \Delta t) + \Delta t \cdot v_x(t - \Delta t) \\&= x(t - 2\Delta t) + \Delta t \cdot (v_x(t - 2\Delta t) + v_x(t - \Delta t)) , \\&= x(0) + \Delta t \sum_{n=1}^N v_x(t - n \cdot \Delta t).\end{aligned}$$

The random walk: mathematical analysis

What is the average position?

$$\langle x(t) \rangle = x_0 + \Delta t \sum_{n=1}^N \langle v_x(t - n \cdot \Delta t) \rangle,$$

where for any time, τ , one has

$$\langle v_x(\tau) \rangle = \frac{1}{5} \left(-\frac{\Delta x}{\Delta t} \right) + \frac{3}{5} \cdot 0 + \frac{1}{5} \frac{\Delta x}{\Delta t} = 0,$$

and therefore

$$\langle x(t) \rangle = x_0.$$

The random walk: mathematical analysis

What is the average displacement?

$$d(t) = \sqrt{\langle (x(t) - x_0)^2 \rangle + \langle (y(t) - y_0)^2 \rangle}$$

Therefore with $d_x^2 = \langle (x(t) - x_0)^2 \rangle$

$$\begin{aligned} d_x^2 &= \Delta t^2 \left\langle \sum_{m=1}^N v_x(t - m\Delta t) \sum_{n=1}^N v_x(t - n\Delta t) \right\rangle, \\ &= \Delta t^2 \sum_{m,n=1}^N \langle v_x(t - m\Delta t) v_x(t - n\Delta t) \rangle. \end{aligned}$$

The random walk: mathematical analysis

Statistical independence

$$\Rightarrow \langle v_x(t - m\Delta t)v_x(t - n\Delta t) \rangle = 0, \quad m \neq n.$$

And for $m = n$

$$\langle v_x^2 \rangle = \frac{1}{5} \left(\frac{\Delta x^2}{\Delta t^2} \right) + \frac{3}{5} \times 0 + \frac{1}{5} \left(\frac{\Delta x^2}{\Delta t^2} \right) = \frac{2\Delta x^2}{5\Delta t^2}.$$

The random walk: mathematical analysis

The sum can be separated in two terms

$$\begin{aligned} d_x^2 &= \Delta t^2 \left(\sum_{\substack{m,n=1 \\ m \neq n}}^N \langle v_x(t - m\Delta t) v_x(t - n\Delta t) \rangle + \sum_{m=1}^N \langle v_x(t - m\Delta t)^2 \rangle \right), \\ &= \sum_{m=1}^N \frac{2\Delta x^2}{5} = N \frac{2\Delta x^2}{5} = t \frac{2\Delta x^2}{5\Delta t}. \end{aligned}$$

The random walk: mathematical analysis

Doing similarly for d_y^2 on gets

$$d = \sqrt{d_x^2 + d_y^2} = \sqrt{t \frac{4\Delta x^2}{5\Delta t}}.$$

Finally by defining the diffusion coefficient $D \equiv \frac{\Delta x^2}{5\Delta t}$

$$d = \sqrt{4Dt}.$$

Equivalent to

$$\partial_t \rho(x, y, t) = D(\partial_x^2 + \partial_y^2) \rho(x, y, t).$$

The random walk: 2D diffusion

Parameters of the simulation

$$t = 100, \Delta x = \Delta t = 1, (x_0, y_0) = (0, 0).$$

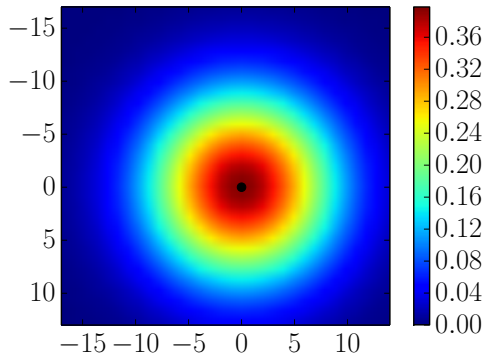
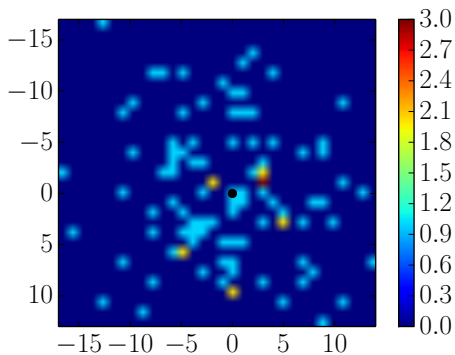
Transport parameters

$$D = \frac{1}{5}, \quad d = \sqrt{80} \cong 8.9443.$$

Let us measure the average position and the average distance at time t for a different number of walkers.

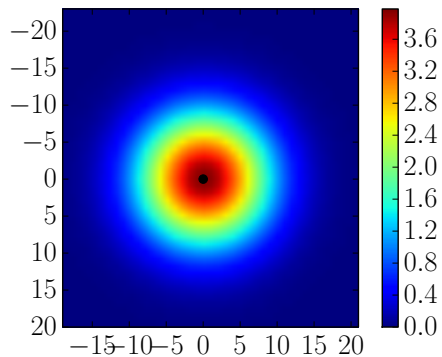
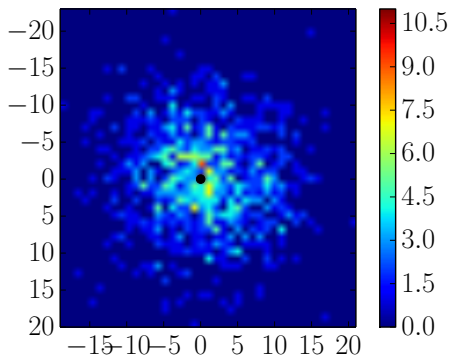
The random walk: $N = 100$

$$\langle (x, y) \rangle = (-0.63, -0.01), \quad d = 9.262$$



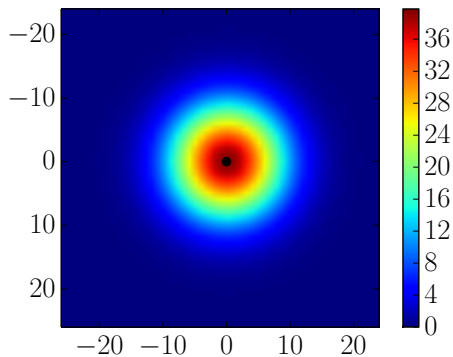
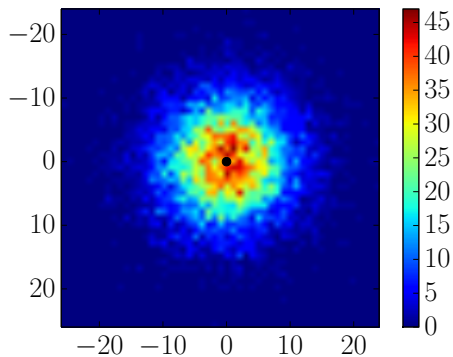
The random walk: $N = 1000$

$$\langle (x, y) \rangle = (0.382, -0.094), \quad d = 9.037$$



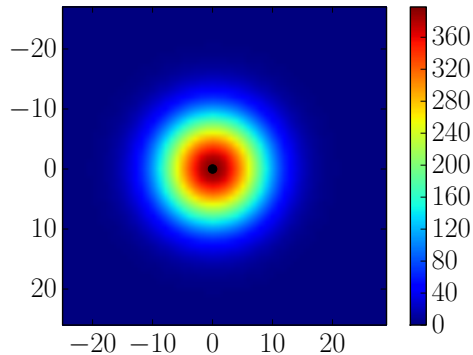
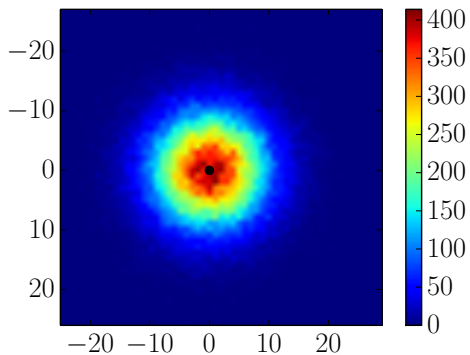
The random walk: $N = 10000$

$$\langle (x, y) \rangle = (0.0034, 0.0335), \quad d = 8.972$$



The random walk: $N = 100000$

$$\langle (x, y) \rangle = (-0.00214, -0.0013), \quad d = 8.938$$



End of module

The random walk

Coming next

Growth of a population

Growth of a population

Growth of a population

- Let us note the number of individuals of a population $P(t)$, and $P(0) = P_0$.
- Only two processes are affecting the number of individuals: the number of births $B(t)$ and the number of deaths $D(t)$.
- The variation of $P(t)$ can be expressed as

$$\dot{P}(t) = B(t) - D(t).$$

- A possible model for births and deaths is given by

$$B(t) = r_b P(t), \quad D(t) = r_d P(t).$$

Growth of a population

Total variation of the population

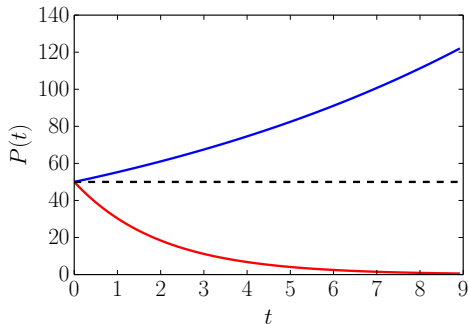
$$\dot{P}(t) = rP(t), \quad r = r_b - r_d.$$

The solution of this equation

$$P(t) = P_0 e^{rt}.$$

Growth of a population

- $r > 0$ exponential growth.
- $r < 0$ exponential decay.
- $r = 0$ constant.



Growth of a population

- Of course an infinite growth of population is not realistic.
- One can add a target “capacity” C to the population by $r \rightarrow 0$ as $P \rightarrow C$

$$r = v \left(1 - \frac{P}{C} \right).$$

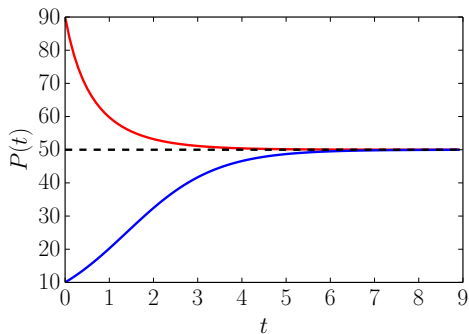
- The model becomes

$$\dot{P} = v \left(1 - \frac{P}{C} \right) P$$

Growth of a population

The solution is a logistic function

$$P(t) = \frac{C}{1 + \frac{C-P_0}{P_0}e^{-vt}}$$



$$C = 50, \quad v = 1, \quad P_0 = 10 \text{ (blue)}, 90 \text{ (red)}.$$

Growth of a population

- $P_0 < C$ growth of population and $P \rightarrow C$.
- $P_0 > C$ decay of population and $P \rightarrow C$.
- Except if $P_0 = 0$ then $P(t) = 0$.

This system has two fixed points: C (attractive) and 0 (repulsive).

End of module

Growth of a population

Coming next

Balance equations

Balance equations I

Balance equations

As shown with the growth of a population example the basic idea is to write a **balance equation**

$$\underbrace{\text{variation of a quantity}}_{\text{ex: } \dot{P}} = \underbrace{\text{creation rate}}_{\text{ex: } B(t)} - \underbrace{\text{destruction rate}}_{\text{ex: } D(t)}.$$

Or to reuse the generic formalism of continuous dynamical systems

$$\dot{s} = f(s) = \text{creation rate} - \text{destruction rate}.$$

Balance equations

For discrete dynamical systems this equation becomes

$$s(t + \Delta t) - s(t) = \Delta t (\text{creation rate} - \text{destruction rate}) .$$

Both formulations are equivalent in the limit $\Delta t \rightarrow 0$ since

$$\lim_{\Delta t \rightarrow 0} \frac{s(t + \Delta t) - s(t)}{\Delta t} = \dot{s} .$$

Discrete balance equations can be directly implemented on a computer.

Lotka–Volterra model (“Prey-Predator”)

Let a be the antelope population and c the cheetah population.

$$\frac{da}{dt} = \underbrace{k_a a(t)}_{(1)} - \underbrace{k_{c,a} c(t) a(t)}_{(2)},$$

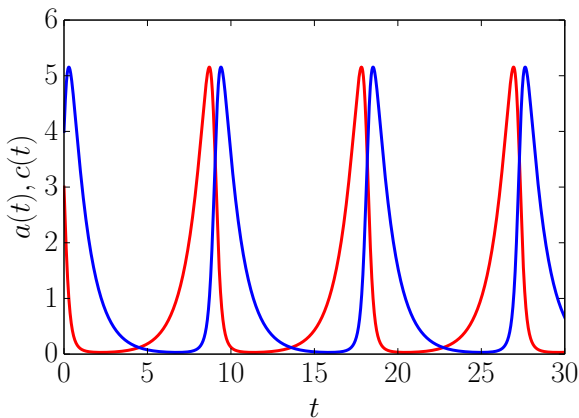
$$\frac{dc}{dt} = -\underbrace{k_c c(t)}_{(3)} + \underbrace{k_{a,c} a(t) c(t)}_{(4)}$$

- The antelopes reproduce exponentially fast (infinite amount of food).
- The antelopes are being eaten by the cheetah proportionally to their chance to meet.
- The cheetahs die exponentially fast of starvation.
- The cheetahs are reproducing proportionally to their chance to eat antelopes.

Lotka–Volterra model (“Prey-Predator”)

Time evolution

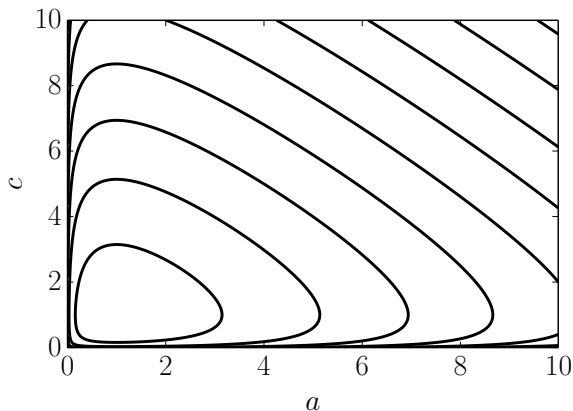
Periodicity



Lotka–Volterra model (“Prey-Predator”)

Parametric plot

Initial condition
sensitivity



End of module

Balance equations I

Coming next

Balance equations II

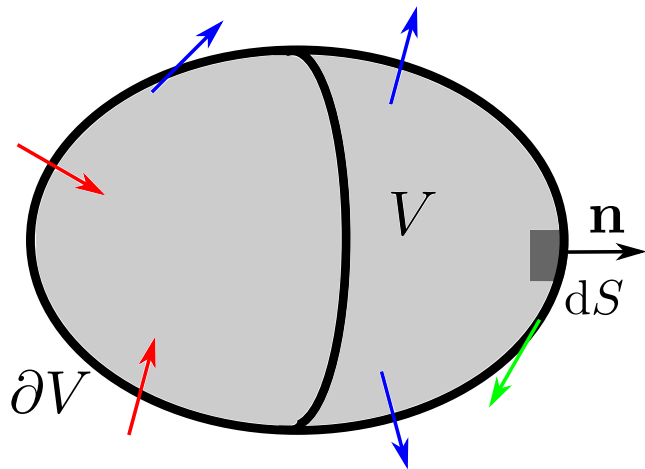
Balance equations II

Space–time dependent equations

- For certain situations time dependence is not sufficient (e. g. weather forecast).
- Necessity to add spatial dependence.
- The balance is now done in a volume $V \in \mathbb{R}^d$ and must not only take into account the destruction/creation processes but also the fluxes through the surface of V , noted ∂V .

The flux through of a quantity is the amount of s crossing ∂V per unit time.

Control volume



The continuity equation

- Let us define $\rho(t, \mathbf{x})$ the volume density of the property one wants to study (mass, electric charge, ...)

$$s(t) = \int_V \rho(t, \mathbf{x}) dV.$$

- Balance equation for $s(t)$ in V reads

$$\dot{s} = - \underbrace{\text{flux}}_{=j} \text{ through surface} + \underbrace{\text{volumic destruction/creation rate}}_{=\Sigma}.$$

The continuity equation

By defining $\Sigma = \int_V \sigma dV$

$$\dot{\Sigma} + \oint_{\partial V} \mathbf{j} \cdot \mathbf{n} dS = \Sigma$$

By using the Gauss–Ostrogradski theorem

$$\int_V \frac{\partial \rho}{\partial t} dV + \int_V \nabla \cdot \mathbf{j} dV = \int_V \sigma dV,$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = \sigma$$

Example: The diffusion equation, $\rho \rightarrow C$

Fick's law $\mathbf{j} = -D\nabla C$, and $\sigma = 0$

$$\frac{\partial C}{\partial t} = D\nabla^2 C,$$

where D is the diffusion coefficient.

Example: The Navier–Stokes equations, $\rho \rightarrow \rho \mathbf{u}$

Momentum flux $\mathbf{j} = \rho \mathbf{u} \mathbf{u} + p \mathbf{I} - \boldsymbol{\tau}$, and $\sigma = 0$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau}.$$

For a Newtonian incompressible fluid

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{u},$$

with ν the kinematic viscosity.

End of module

Balance equations II

Coming next

Integration of ordinary differential
equations

Integration of ordinary differential equations

Integration of ordinary differential equations

Let us define a one-dimensional differential equation

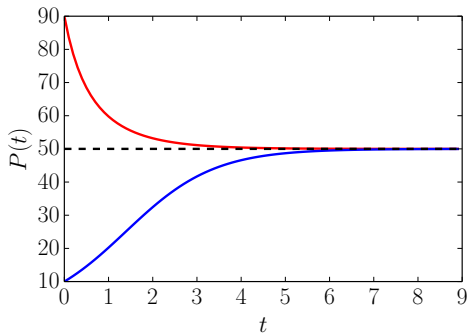
$$\dot{s} = f(s, t), \quad t_0 \leq t \leq t_f, \text{ and } s(t = t_0) = s_0.$$

where f is a function of s and t , and s_0 is a prescribed initial condition. Depending on the form of f , $s(t)$ may be difficult to obtain analytically.

Example: Growth of a population

$$\dot{s} = f(s, t), \quad f(s, t) = v \left(1 - \frac{s}{C} \right) s.$$

$$s(t) = \frac{C}{1 + \left(\frac{C-s_0}{s_0} \right) e^{-vt}}$$



Explicit Euler scheme, $\dot{s} = f(s, t)$

Find approximate solution at $t_1 = t_0 + \Delta t$ (Taylor exp.)

$$s(t_0 + \Delta t) = s(t_0) + \Delta t \cdot \dot{s}(t_0) + \underbrace{\mathcal{O}(\Delta t^2)}_{\text{error}}$$

With the definition of the differential equation we find

$$s(t_1) = s(t_0) + \Delta t \cdot f(s, t_0).$$

Explicit Euler scheme (continued)

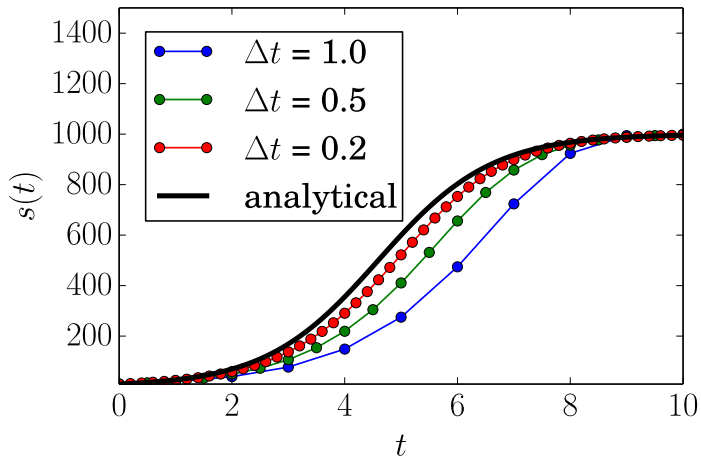
Iteratively one finds the explicit or forward Euler scheme

$$s(t_{n+1}) = s(t_n) + \Delta t \cdot f(s, t_n), \quad t_{n+1} = t_n + \Delta t.$$

Remarks

- It looks a lot like a discrete dynamical system!
- $s(t_{n+1})$ depends **explicitly** on $s(t_n)$.
- Straightforward to implement on a computer.

Example: growth of a population



End of module

Integration of ordinary differential
equations

Coming next

Error of the approximation

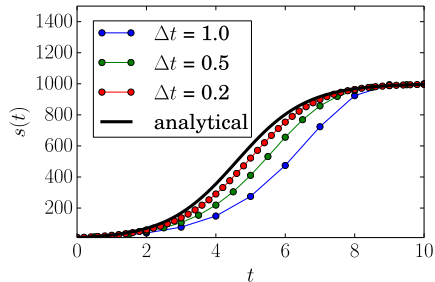
Error of the approximation

Error of the approximation

Evaluation of the error

$$E(\Delta t) = \sqrt{\frac{1}{N+1} \sum_{i=0}^N (s(t_i) - s_{\Delta t}(t_i))^2},$$

with $N = (t_f - t_0)/\Delta t$



Remark

- If no analytical solution exists one can replace $s(t_i) \rightarrow s_{\min(\Delta t)}(t_i)$.

Evaluation of the error

Evaluation of the error, $s_i = s(t_i)$

$$s_1 = s_0 + \Delta t \cdot f(s_0, t_0) + \mathcal{O}(\Delta t^2),$$

$$s_2 = s_1 + \Delta t \cdot f(s_1, t_1) + \mathcal{O}(\Delta t^2),$$

$$\Rightarrow s_2 \cong s_0 + \Delta t \cdot \{f(s_0, t_0) + f[s_0 + \Delta t \cdot f(s_0, t_0), t_0 + \Delta t]\} + 2\mathcal{O}(\Delta t^2).$$

The error accumulates: after $2\Delta t$

$$s(t_0 + 2\Delta t) - s_{\Delta t}(t_0 + 2\Delta t) \sim 2 \times \mathcal{O}(\Delta t^2).$$

Evaluation of the error

Defining $E_i = s(t_i) - s_{\Delta t}(t_i)$, we have

$$E_0 = s(t_0) - s_{\Delta t}(t_0) = 0, \dots,$$

$$E_N = s(t_N) - s_{\Delta t}(t_N) = N\mathcal{O}(\Delta t^2).$$

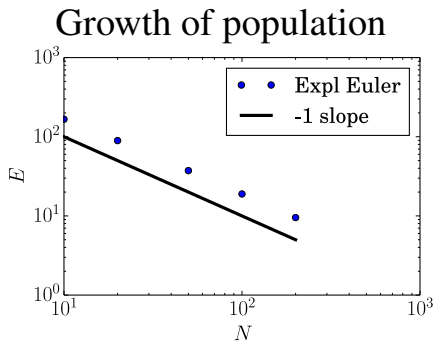
Therefore

$$E = \sqrt{\frac{1}{N+1} \sum_{i=0}^N E_i^2} \sim \sqrt{\frac{\mathcal{O}(\Delta t^4)}{N+1} \sum_{i=0}^N i^2} \sim \sqrt{\Delta t^4 N^2} \sim \mathcal{O}(\Delta t),$$

where we used that $N = (t_f - t_i)/\Delta t \sim \mathcal{O}(\Delta t^{-1})$.

Order of the scheme

- The forward Euler scheme is of **order** 1, since $E \sim \mathcal{O}(\Delta t^1)$.
- Δt is divided by a factor $M \Rightarrow$, E is decreased by a factor M .
- A scheme is of order k if $E \sim \mathcal{O}(\Delta t^k)$.



End of module

Error of the approximation

Coming next

Implicit Euler scheme

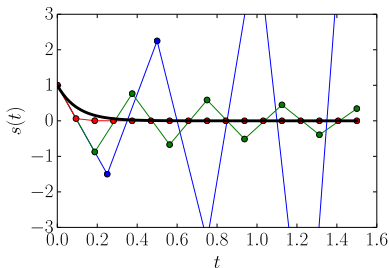
Implicit Euler scheme

Stability of explicit schemes

Example: $\dot{s} = -10s(t)$, $t_0 = 0$, $t_f = 1.5$, $s_0 = 1$.

Solution: $s = s_0 \exp(-10t)$. Euler: $s(t + \Delta t) = s(t) - 10\Delta t \cdot s(t)$.

Explicit Euler scheme



- Difficult to solve **stiff** problems with large Δt .
- Since only information about t_{n-1} is known when going to t_n “too big” jumps are possible.

The implicit Euler scheme

Instead of s_{j+1} we approximate s_{j-1}

$$s_{j-1} = s_j - \Delta t \cdot f(s, t_j) + \mathcal{O}(\Delta t^2)$$

Our differential equation is now approximated by the *backward Euler scheme*

$$s_j = s_{j-1} + \Delta t \cdot f(s_j, t_j) \Leftrightarrow \boxed{s_{j+1} = s_j + \Delta t \cdot f(s_{j+1}, t_{j+1})}.$$

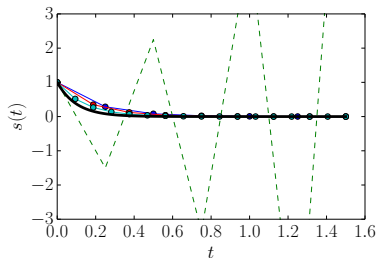
This class of approximation is called *implicit*.

Implicit Euler scheme (continued)

Example: $\dot{s} = -10s(t)$, $t_0 = 0$, $t_f = 1.5$, $s_0 = 1$.

Solution: $s = s_0 \exp(-10t)$.

Implicit Euler scheme



- Implicit scheme

- Explicit scheme

$$s_{j+1} = s_j - 10\Delta t s_{j+1}, \quad s_{j+1} = s_j(1 - 10\Delta t).$$

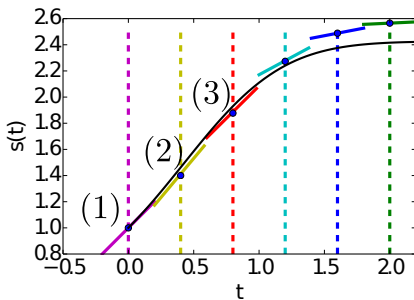
$$s_{j+1} = s_j / (1 + 10\Delta t).$$

- Instability solved.

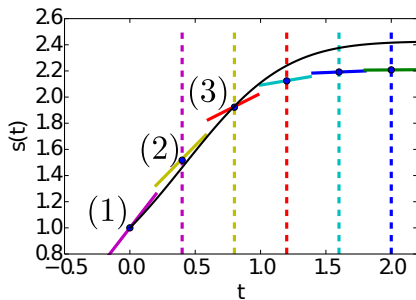
Explicit vs Implicit (continued)

Graphical interpretation

Explicit



Implicit



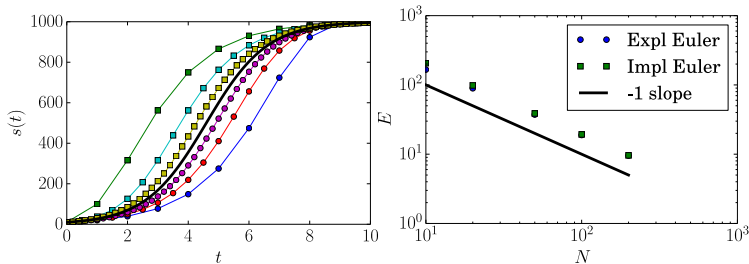
Explicit vs Implicit

Explicit

- Explicit equation to solve
- Conditionally stable (on stiff problems)
- Simple implementation

Implicit

- Implicit equation to solve
- Unconditionally stable
- Difficult implementation



Explicit/Implicit solution (left) and error (right) on the population growth problem.

End of module

Implicit Euler scheme

Coming next

Numerical integration of partial
differential equations

Numerical integration of partial differential equations

The diffusion equation

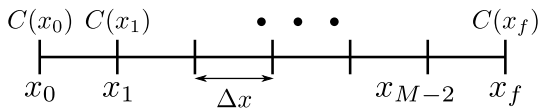
In 1D the diffusion equation reads

$$\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2}, \quad t \in [t_0, t_f], \quad x \in [x_0, x_f],$$

with the following spatial boundary conditions $C(x = x_0, t) = C_0$ et $C(x = x_f, t) = C_1$ and initial condition $C(x, t_0) = C_x$.

Not only time must be discretized but also space.

The diffusion equation: space discretization



- The physical space is divided in $M + 1$ equidistant points with $M = (x_f - x_0)/\Delta x$.
- The set of points is defined such as $x_{i+1} = x_i + \Delta x$ and $x_f = x_M$.
- The concentration is defined on each point with $C_i \equiv C(x_i)$.
- The time dependence is understood here.

The diffusion equation: space discretization

The Taylor expansion of C_{i+1} and C_{i-1} to second order reads

$$C_{i+1} = C_i + \Delta x \frac{\partial C_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C_i}{\partial x^2},$$
$$C_{i-1} = C_i - \Delta x \frac{\partial C_i}{\partial x} + \frac{\Delta x^2}{2} \frac{\partial^2 C_i}{\partial x^2}.$$

By summing these equations one gets ($x_i \in [x_1, \dots, x_{M-1}]$)

$$\frac{\partial^2 C_i}{\partial x^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2}$$

The diffusion equation: space discretization

The discretization of the Laplacian leads to

$$\frac{\partial C_i(t)}{\partial t} = D \frac{C_{i+1}(t) - 2C_i(t) + C_{i-1}(t)}{\Delta x^2}.$$

By defining $\mathbf{C}(t) = (C(x_0, t), C(x_1, t), \dots, C(x_M, t))^T$ and \mathbf{A} as

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 0 & 0 & \dots & 0 \\ 1 & -2 & 1 & 0 & \dots & 0 \\ 0 & 1 & -2 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & 1 & -2 & 1 \\ 0 & \dots & \dots & \dots & 0 & 1 \end{pmatrix}$$

Remark

- The first and last lines of \mathbf{A} correspond to boundary conditions.

The diffusion equation: time discretization

We can now rewrite the diffusion equation under a matrix form

$$\frac{\partial \mathbf{C}(t)}{\partial t} = \frac{D}{\Delta x^2} \mathbf{A} \mathbf{C}(t).$$

Explicit time discretization

$$\frac{\mathbf{C}(t_{i+1}) - \mathbf{C}(t_i)}{\Delta t} = \frac{D}{\Delta x^2} \mathbf{A} \mathbf{C}(t_i).$$

Implicit time discretization

$$\frac{\mathbf{C}(t_{i+1}) - \mathbf{C}(t_i)}{\Delta t} = \frac{D}{\Delta x^2} \mathbf{A} \mathbf{C}(t_{i+1}).$$

The diffusion equation: time discretization

Explicit time discretization

$$\mathbf{C}(t_{i+1}) = \left(\frac{\Delta t D}{\Delta x^2} \mathbf{A} + \mathbf{I} \right) \mathbf{C}(t_i).$$

Implicit time discretization

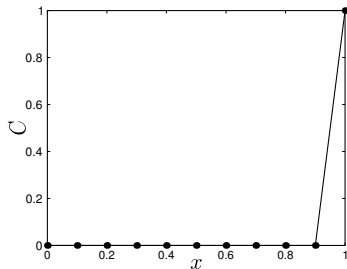
$$\mathbf{C}(t_{i+1}) = \left(-\frac{\Delta t D}{\Delta x^2} \mathbf{A} + \mathbf{I} \right)^{-1} \mathbf{C}(t_i).$$

Remarks

- Implicit scheme needs matrix inversion (it is an art!) but stable.
- Explicit scheme easy to implement but unstable (CFL).

Numerical example

Initial condition

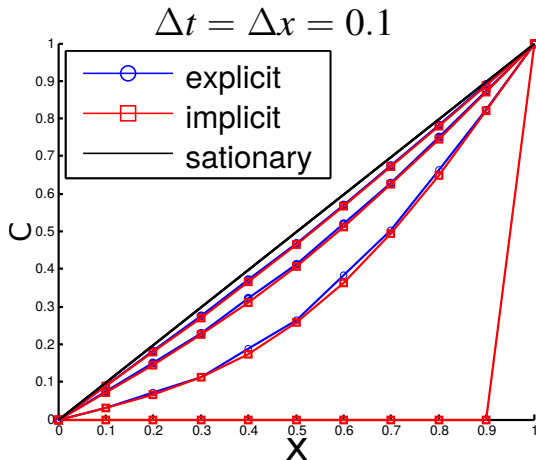


Boundary conditions

$$C(x_0, t_i) = 0, \quad C(x_f, t_i) = 1, \forall t_i.$$

For $t \rightarrow \infty$ admits a stationary solution.

Numerical example



End of module

Numerical integration of partial
differential equations

End of Week 3

Thank you for your attention!