2. Initial value problems

Modeling with ODEs

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Introduction

- *Differential equations* is the most widely used mathematical structure of mechanistic models.

- They are equations that involve derivatives of an unknown function.

- They help to understand the processes within the system

Introduction

- Classification:
  - *Ordinary Differential Equation (ODE)*: involve only the derivative of one variable.
  - *Partial Differential Equations (PDE)*: involve the derivative of more than one variable.

Ordinary Differential Equations

- Deffinition:

$$f\left(x, y, y', y'', \ldots, y^{(n)}\right) = 0$$

Where $\mathrm{y} = f(x)$

Order of an ODE

- Maximum order of the derivatives:
  - $y'' + y' \cdot \sin(x) = 2x$ → Second order
  - $y^{(n)} = f\left(x, y, y', y'', \dots, y^{(n-1)}\right)$ → n-order
  - $T' = k(T - T_a), T = T(t), k, T_a \in \mathbb{R}$ → First order

Motivation

- Where do EDOS come from?
- Origin of ODEs
  - Why do they appear?
  - How are they deduced?
  - Where do they come from?

- They appear from observable phenomena, from experimentation
- We can generally calculate or estimate the rates of change of certain quantities but not the quantities.

Example: Maltus population dynamics

- **Maltus**: The rate of change of a population with respect to time is proportional to the size of the population (considering birth and mortality rates constants).

- Be $P = P(t)$ the population size in an instant $t,$ its rate of change with respect to time will be:

$$P' = P'(t) = \frac{d\left(P(t)\right)}{dt}$$

- Therefore, according to Malthus, the rate of change is proportional to the size of the population:

$$\boxed{P'(t) = k \cdot P(t), k \in \mathbb{R}}$$

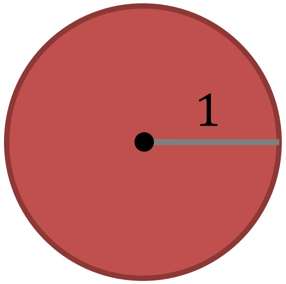
$$Differential\ equation\ of\ first\ order$$

General idea of ODEs

- What is π?

$$\pi = 3.1415926535897932384626433832795028841971693993\ldots$$

$$\pi = 4 \cdot \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1}$$



General idea of ODEs

- What is e?

$$e = 3.14159265358979323846264338327950288419716939937...$$

$$e = \sum_{n=0}^{\infty} \frac{x^n}{n!}$$

$$f(t) = e^t$$

$$f'(t) = e^t$$

$$f(0) = 1$$

Ordinary Differential Equations

Remember

- Deffinition:

$$f\left(x, y, y', y'', \ldots, y^{(n)}\right) = 0$$

Where $\mathrm{y} = f(x)$

Is there a unique solution?

ODEs as function generators

- What is the function defined by these equations?

$$f''(t) = -f(t)$$

$$f(0) = 1$$

$$f'(0) = 0$$

ODE General solution

- The general solution of $\mathrm{F}(x, y, y', y'', \dots, y^{(n)}) = 0$ is a family of functions

$$y = f(x, C_1, C_2, \dots, C_n)$$

Where $C_i \in \mathbb{R}$

ODEs as function generators

- What is the function defined by these equations?

$$f''(t) = -f(t)$$

$$f(0) = 1$$

$$f'(0) = 0$$

Example: Maltus population dynamics

$$P'(t) = k \cdot P(t), k \in \mathbb{R}$$

$$\frac{dP}{dt} = k \cdot P$$

$$\frac{dP}{P} = k \cdot dt \Rightarrow \int \frac{1}{P} \cdot dP = \int k \cdot dt$$

$$\int \frac{1}{P} \cdot dP = \ln(P) + C_1, \int k \cdot dt = k \cdot t + C_2$$

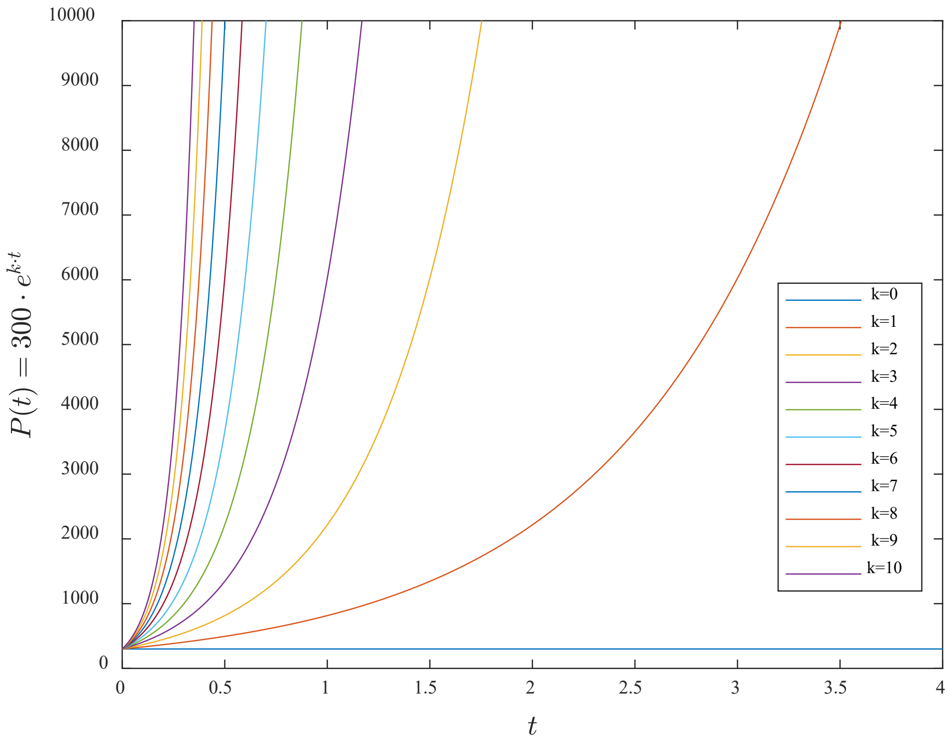
$$\ln(P) = k \cdot t + C_3 \Rightarrow P = e^{k \cdot t + C_3} = C \cdot e^{k \cdot t}$$

Example: Maltus population dynamics

- If the initial population was 300:

$$P(0) = 300 = C \cdot e^{k \cdot 0} \Rightarrow C = 300$$

$$P(t) = 300 \cdot e^{k \cdot t}$$



Basic concepts

- **First-order ODEs**
  - Let $\Omega \subset \mathbb{R}^2, F: \Omega \to \mathbb{R}$ a continuous function. Then:

$$y'(t) = F\big(t, y(t)\big)$$

is a first-order ODE in the unknown function $y(t)$. A function $y: [a, b] \to \mathbb{R}$ is called ***a solution of the ODE*** if this equation is satisfied for every $t \in [a, b] \subset \mathbb{R}$

Basic concepts

- **Autonomous:** the ODE does not depend on t explicitly.
  - $y' = F(y(t)) \rightarrow Autonomous$. E.g. $y' = y$
  - $y' = F(y(t), t) \rightarrow Non\ autonomous$. E.g. $y' = y \cdot e^{-t}$

Basic concepts

- **The initial value problem**

  Let $\Omega \subset \mathbb{R}^2, F: \Omega \to \mathbb{R}$ a continuous function and $y_0 \in \mathbb{R}$. Then:

$$y'(t) = F\big(t, y(t)\big)$$

$$y(a) = y_0$$

is an *initial value problem* for the ODE equation. A function $y: [a, b] \to \mathbb{R}$ is called ***a solution of the ODE*** if both equations are satisfied for every $t \in [a, b] \subset \mathbb{R}$

Basic concepts

- **Linear versus nonlinear**
  - A linear ODE is a linear polynomial in the unknown function

$$y^{(n)} = b(x) + a_0(x) \cdot y + a_1(x) \cdot y' + \cdots + a_{n-1}(x) \cdot y^{(n-1)}$$
$$= b(x) + \sum_{i=0}^{n-1} a_i(x) \cdot y^{(i)}$$

  - Example:
    - Body temperature
    - Clock alarm temperature

Basic concepts

- **Closed form vs. Numerical solutions**
  - Closed form: (otherwise known as analytical solution) Is a solution of the ODE in terms of "well-known" equations. Most ODEs cannot be solved in this way.
  - Numerical form: Appropriate computer algorithms are used to obtain approximations of the ODE solutions.

Numerical solution of ODEs

- **Implicit and explicit solutions**:
  - **Explicit**: Methods that calculate the value of the system at a later time from the state of the system at the current time.
$$Y(t + \Delta t) = F(Y(t))$$
  - **Implicit**: Methods that find a solution to $Y(t + \Delta t)$ by solving an equation involving the current state of the system and the later one.
$$G(Y(t), Y(t + \Delta t)) = 0$$
  - **Operator splitting**: the differential operator is rewritten as the sum of two complementary operators.
$$Y(t + \Delta t) = G\big(Y(t + \Delta t)\big) + F(Y(t))$$

Definition of derivative

$$\frac{df(t)}{dt} = \lim_{\Delta t \to 0} \frac{f(t + \Delta t) - f(t)}{\Delta t}$$

- If Δt is close to 0 we can approximate:

$$\frac{df(t)}{dt} \approx \frac{f(t + \Delta t) - f(t)}{\Delta t} \rightarrow f(t + \Delta t) \approx f(t) + \frac{df(t)}{dt} \cdot \Delta t$$

- If $\frac{df(t)}{dt}$ is known, and the value of $f(0)$ is also known, we can calculate the value of $f(t)$

- This method is called ***Fordward Euler*** and is an explicit method: the value in $t + \Delta t$ is calculated based on the derivative in t (a previous instant of time)

Example: Gravity problem

- **Explicit**

$$v'(t) = \frac{dv(t)}{dt} = g, \qquad x'(t) = \frac{dx(t)}{dt} = v(t)$$

$$v(t + \Delta t) = v(t) + \Delta t \cdot v'(t) = v(t) + \Delta t \cdot g$$

$$\begin{aligned} x(t + \Delta t) = x(t) + \Delta t \cdot x'(t) = \\ = x(t) + \Delta t \cdot v(t) \end{aligned}$$

Example: Gravity problem

- **Explicit**

$$v' = \frac{dv}{dt} = g, \qquad x' = \frac{dx}{dt} = v(t), \qquad v(0) = 0, \qquad x(0) = 10$$

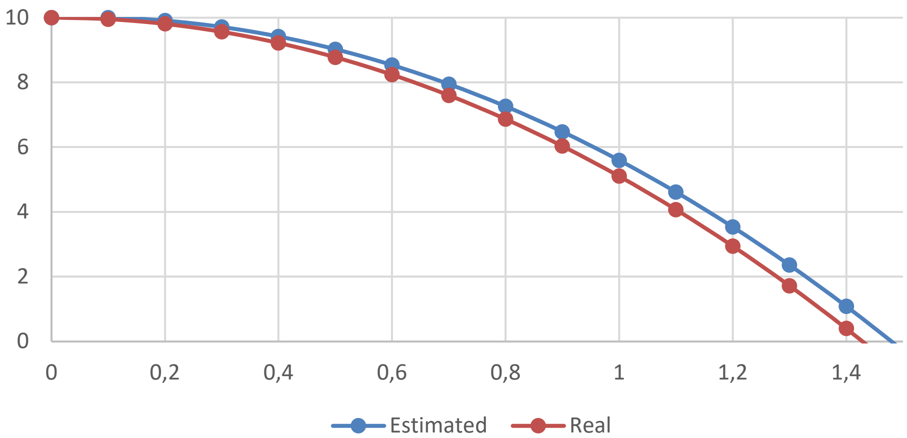
– Step 0:
  - $v'(0) = g,\ v(0) = 0$
  - $x'(0) = v(0),\ x(0) = 10$

– Step 1:
  - $v(\Delta t) = v(0) + \Delta t \cdot v'(0) = \Delta t \cdot g$
  - $x(\Delta t) = x(0) + \Delta t \cdot x'(0) = 10$

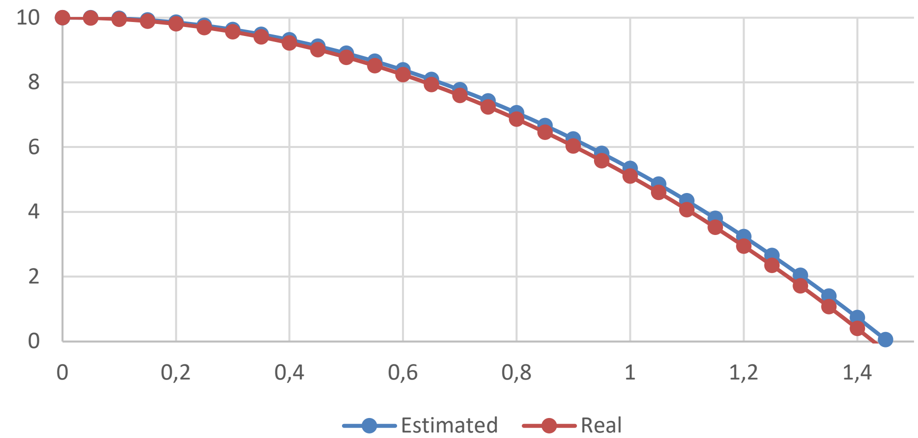
– Step 2:
  - $v(2\Delta t) = v(\Delta t) + \Delta t \cdot v'(\Delta t) = 2\Delta t \cdot g$
  - $x(2\Delta t) = x(\Delta t) + \Delta t \cdot x'(\Delta t) = 10 + \Delta t^2 \cdot g$

Example: Gravity problem

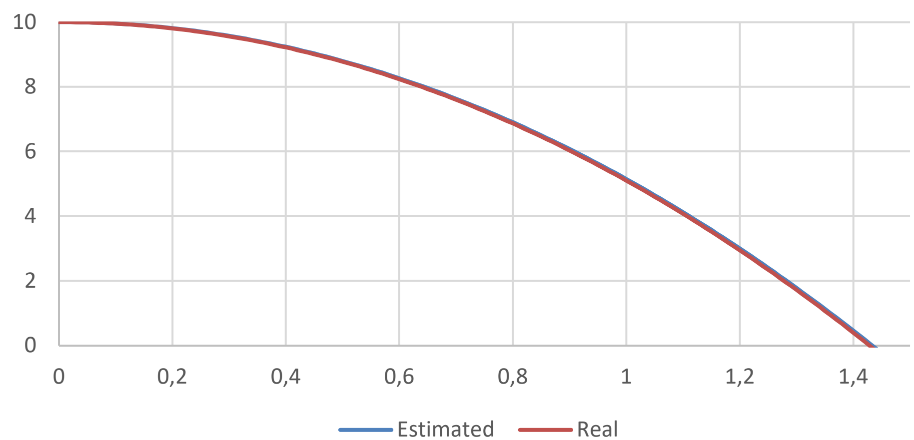
$\Delta t = 0.1$



$\Delta t = 0.05$



$\Delta t = 0.01$



Forward Euler Method

- The method used in the example is the Forward Euler Method

- The value of the state variables in an instant t is calculated with the information of the system in the previous instant (t-Δt)

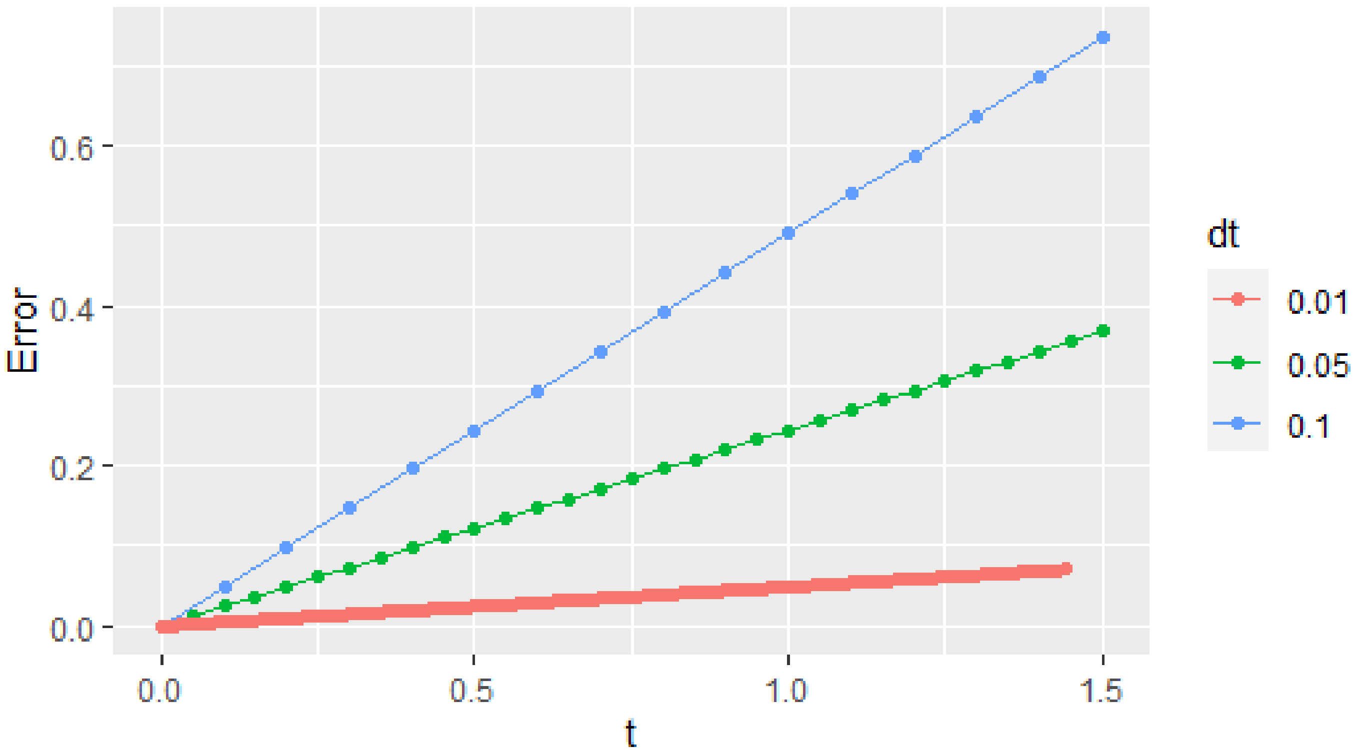
$$y(t) = y(t - \Delta t) + y'(t - \Delta t) \cdot \Delta t$$

- **Explicit** method.

Example: Gravity problema (cont)

Evaluating the (absolute) error of the approximation as:

$$E = |y - \hat{y}|$$



Forward Euler Method

- **Order of convergence**: How fast a method converges towards the exact solution if the stepsize (h) is decreased towards 0.

- Forward Euler Method order of convergence is 1:

$$y_1 = y(0) + h \cdot y'(0)$$

$$y(h) = y(0) + h \cdot y'(0) + \frac{1}{2}h^2 \cdot y''(0) + O(h^3)$$

$$y(h) - y_1 = \frac{1}{2}h^2 \cdot y''(0) + O(h^3)$$

From this we can see that:

$$Error \sim h^2 \;\&\; Stepsize \sim \frac{1}{h} \rightarrow Order = h^1$$

Exercise:

Considering the first order ODE:

$$y' = -15\, y$$
$$y(0) = 1$$

This is an example of what is known as **Stiff equation** because its numerical solution is unstable unless a small step size is used.

a) Analytically obtain its solution.
b) Write an R script for obtaining the numerical solution using the Euler Method with a $\Delta t = 0.01$ and $0 \leq t \leq 1$. Analyze the error and convergence of the method for this setting.
c) Modify $\Delta t = 1/8$ and repeat the calculations, draw your own conclusions.

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