

Computational Biology

Chapter 1: Discrete-time models

Adérito Araújo

CMUC, University of Coimbra, Portugal



UNIVERSIDADE D
COIMBRA

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Course Overview

Introduction and Syllabus

Computational Biology

Adérito Araújo (alma@mat.uc.pt)

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What is Computational/Mathematical Biology?

- ▶ **What can biology offer mathematics and computation?**
Biological models offer a seemingly endless supply of challenging and interesting nonlinear problems to solve. These nonlinear problems can provide a testing ground for applied mathematical and computational methods, and generate the impetus to develop new mathematical and computational methods and approaches.
- ▶ **What mathematics and computation offer to biology?**
Mathematics and computation can help solve a growing problem in biological research. Data collection, varying from gene sequencing to remote sensing via satellites, is now inundating biologists with complex patterns of observations. It is the analysis of mathematical models that allow us to formalize the cause and effect process and tie it to biological observations.



Course topics

1. Discrete-Time Models
 - 1.1 Malthus, logistic and Ricker models
 - 1.2 Linear stability analysis
 - 1.3 Systems of discrete-time equations
 - 1.4 Age structured population
2. Ordinary Differential Equations
 - 2.1 Scalar equations
 - 2.2 Systems of equations
 - 2.3 Qualitative behaviour of a system of ODEs
 - 2.4 Numerical methods for ODEs
3. Partial Differential Equations
 - 3.1 Reaction diffusion equations
 - 3.2 Critical size domain
 - 3.3 Travelling waves
 - 3.4 Numerical methods for PDEs



References

[1] Gerda de Vries, Thomas Hillen, Mark Lewis, Johannes Müller, Birgitt Schönfich, *A Course in Mathematical Biology*, SIAM, 2006 (Chapters 2-4).

[2] Ruthe E. Baker, *Mathematical Biology and Ecology Lecture Notes*, University of Oxford, 2011.

[3] Nicholas F.. Britton, *Essential Mathematical Biology*, Springer, 2003.

[4] Brian Ingalls, *Mathematical Modelling in Systems Biology: An Introduction*, University of Waterloo, 2018.

[5] James D. Murray, *Mathematical Biology*, vols. I and II, Springer, 2003.

[6] Eduardo Sontag, *Lecture Notes on Mathematical Systems Biology*, Rutgers University, 2015.



Homework and grading

- ▶ Homework assignments
 - ▶ All homework assignments are due in 1 week
 - ▶ You can discuss course materials and homework problems with others, but you must write your answers completely independent
 - ▶ Do NOT copy solutions from any source. Do NOT share your solutions to others
- ▶ Online meetings
 - ▶ You are expected to attend and participate in all the online meetings
- ▶ Grading
 - ▶ Homework assignments: 80%
 - ▶ Online meetings: 20%



Motivation

Epidemic model SIR

Computational Biology

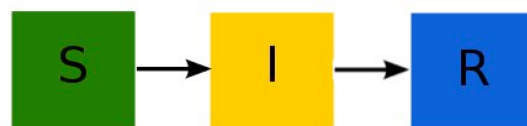
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Epidemic model SIR

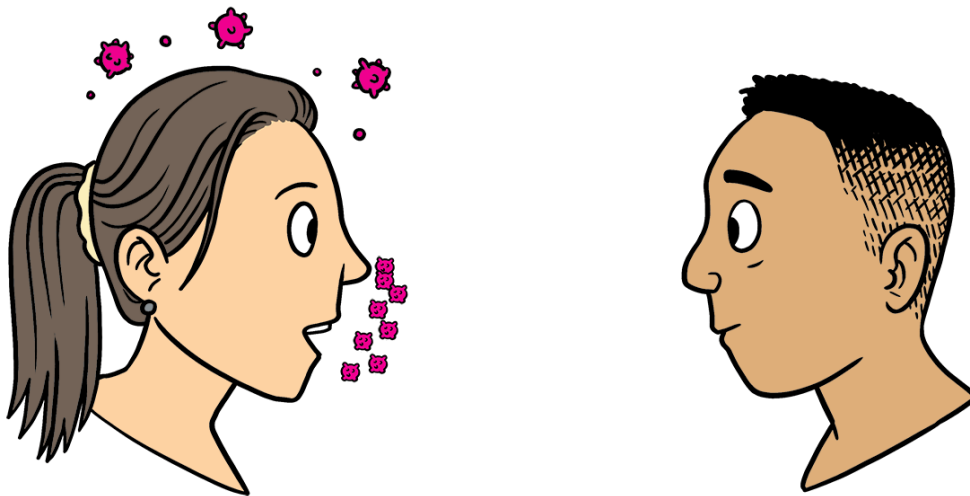
Epidemic model for the spread of an infectious disease (e.g. *influenza* or *covid19*)



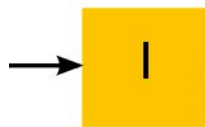
1. Identify important quantities (**dependent variables**) to keep track of: S = susceptible; I = infected; R = recovered;
2. Identify the **independent variables** such of time, space, age, and so on: t = time;
3. Quantify the **transactions and/or interactions** between these classes.



Transmission by contact



Simplified epidemic model I (infected)



1. The dependent variable is the number of infected individuals I .
2. The independent variable is time t .
3. Assume that
 - ▶ E is the average number of people someone infected is exposed per unit time (typically a day);
 - ▶ p is the probability each exposure becoming an infection.

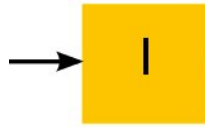
Then, if t represents the actual time (e.g. day)

$$I(t+1) = I(t) + \underbrace{pE}_{r} I(t) = (1+r)I(t),$$

where r represents the **rate of infection**.



Simplified epidemic model I (infected)



Let Δt denote a time period (e.g. a fraction of a day). Then

$$I(t + \Delta t) = I(t) + \Delta t r I(t) \Rightarrow \frac{I(t + \Delta t) - I(t)}{\Delta t} = r I(t).$$

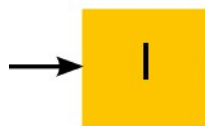
Since r is constant, taking the limit as $\Delta t \rightarrow 0$, we have

$$\frac{dI}{dt}(t) = r I(t).$$

Note: The growth rate is proportional to the number of infected individuals.



Discrete and continuous models



Chapter 2 [1]: Discrete-time model ($t = n\Delta t$)

$$I_{n+1} = (1 + r\Delta t)I_n \stackrel{?}{\Rightarrow} I_n = I_0 (1 + r\Delta t)^n = I_0 \left(1 + \frac{rt}{n}\right)^n, \quad n \geq 1.$$

Chapter 3 [1]: Continuous-time model (ODE)

$$\frac{dI}{dt}(t) = r I(t) \stackrel{?}{\Rightarrow} I(t) = I(0)e^{rt}.$$

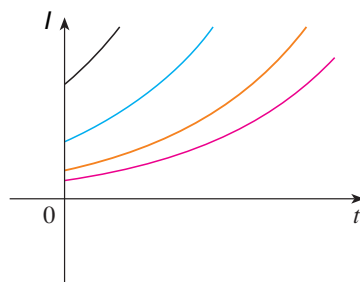


Figure: $I(t) = Ce^{rt}$, with $r > 0$, $t \geq 0$, for different values of C .



Exponential growth: COVID-19 Portugal (March 2020)

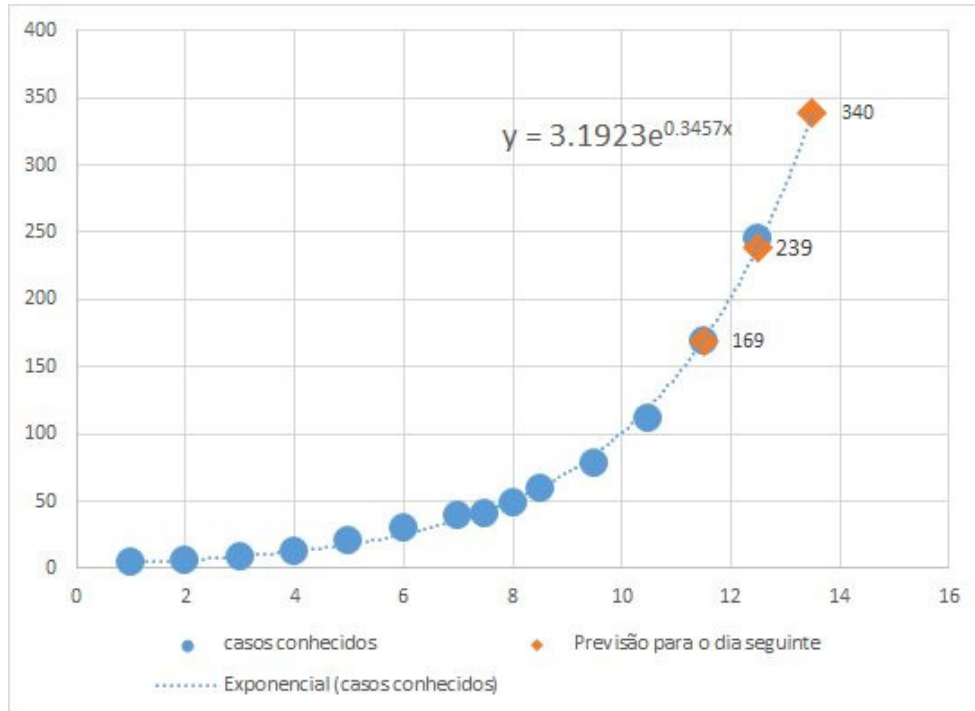


Figure: Expresso, March 16, 2020.



COVID-19 Portugal: exponential or logistic growth?

