Handout on

Mathematics for EES students - Discrete-time modelling

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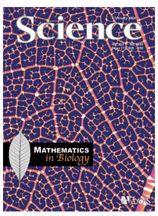
Contents

1 Introduction

Goals of this lecture

- Learn/Remember basic mathematics and modelling used in the EES Master
- Learn to know each other

Mathematics in Biology



Feb. 2004

- Plea from W. Bialek (Physicist) and D. Botstein (Molecular biologist) for mathematics and physics to be more integrated in biology curricula.
- Galileo Galilei: "The book of nature is written in the language of mathematics."
- John Maynard Smith (book Evolutionary genetics): "If you can't stand algebra, keep out of evolutionary biology."
- Robert M. May warns: misuses of maths in biology when biologists do not have enough maths knowledge.

Topics

- Sums and Products
- Equations

- Functions, Derivatives and Integrals
- Modelling: Discrete Processes
- Modelling: Continuous Processes
- Statistics

Organization

For each session we will have:

- A handout
- An exercise sheet (corresponding to the lecture we covered during the last session)

What we expect from you:

- Come to the lecture session; ask questions if something is not clear
- exercise session: present your solutions for the exercise sheet

2 Mathematic modelling in Biology

Mathematical models in EES

Examples of models used in Ecology, Evolution or Systematics.

- Ecology: Lotka–Volterra model for predator–prey population size dynamics
- Evolution: Evolution of allele frequencies depending on mutation, selection and genetic drift (Wright–Fisher model).
- Systematics: Sequence-evolution models for the reconstruction of phylogenies (Jukes–Cantor, HKY, GTR,...).

What is a mathematical model?

"All models are wrong, but some are useful." G. Box

- A model is a representation of a biological system using mathematics formalism.
- A model is a simplification of the reality.
- Thus a model is built on a series of decisions *or assumptions.*
- In general, the more abstract the model is, the easier it is to handle but the more imprecise it becomes.
- The art of modelling is to find the essential aspects of a biological system. This requires a good biological and mathematical knowledge.

Purposes of mathematical modelling

Understanding a mechanism or phenomenon $\rightsquigarrow$ simple model

Check whether an explanation really works $\rightsquigarrow$ may require a more complex model

Making predictions $\rightsquigarrow$ more complex models, computer simulations

Data analysis and statistical testing $\rightsquigarrow$ more or less complex models, depending on statistical/computational methods and size and structure of data to be explained

3 Geometric growth

Discrete-time modelling

- Follow the evolution of a population with discrete generations
- The population size X at generation n is noted X_n.
- The X_n build a mathematical sequence.
- If this sequence is iterative, there is a function f so that $X_{n+1} = f(X_n)$ for all n.

Reminder: functions

A function $f : D \to \mathbb{R}$ assigns to each $x \in D$ one and only one $f(x) \in \mathbb{R}$.

Some functions can be represented by an algebraic expression or have a famous name, for example:

$$\begin{aligned} g : \mathbb{R} &\to \mathbb{R} \\ x &\mapsto 3x^2 + x - 3 \end{aligned}$$

$$\begin{aligned} h : \mathbb{R} \setminus \{0\} &\to \mathbb{R} \\ x &\mapsto \frac{1}{x} \end{aligned}$$

$$\begin{aligned} \exp : \mathbb{R} &\to \mathbb{R}_{>0} \\ x &\mapsto e^x \end{aligned}$$

$$\begin{aligned} \sin : \mathbb{R} &\to [-1; 1] \\ x &\mapsto \sin(x) \end{aligned}$$

$$\begin{aligned} f(x) &= a + bx \qquad \text{(affine-linear function} \\ &\quad\ \text{with intercept } a \text{ and slope } b) \end{aligned}$$

$$\begin{aligned} \ell(x) &= 2 \cdot (x-3)^2 + 5 \\ &= 2x^2 - 12x + 23 \qquad \text{(parabola)} \end{aligned}$$

Reminder: exponential and logarithm

$a^n = b \Leftrightarrow n = \log_a b = \frac{\ln b}{\ln a}$

Properties:
$a^0 = 1, \qquad a^{b+c} = a^b \cdot a^c, \qquad a^{bc} = (a^b)^c$

$\exp(x) = e^x$ with $e \approx 2.71828$

$\ln(\exp(x)) = \exp(\ln(x)) = x$ inverse function

Properties: $\log_a 1 = 0, \qquad \log_a(bc) = \log_a b + \log_a c, \qquad \log_a(b^n) = n \log_a(b)$

Geometric growth model

Example: population growth of a bird population on an island

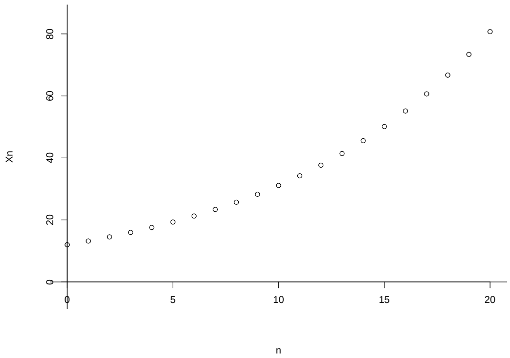
$X_{n+1} = X_n + X_n \cdot b - X_n \cdot d = X_n \cdot (1 + b - d)$
with $b =$ birth rate and $d =$ death rate

Define $r = 1 + b - d =$ growth ratio,
you have a linear process $X_{n+1} = r \cdot X_n$

$\Rightarrow X_n = r^n \cdot X_0$

Graphical representation

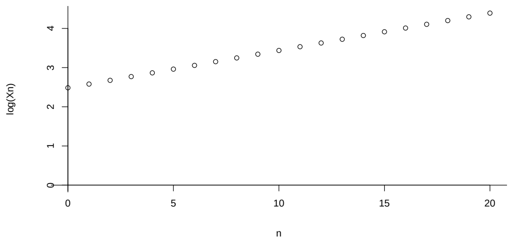
For $X_0 = 12$ and $r = 1.1$



Graphical representation

And on the log scale:

$\log X_n = \log(r^n \cdot X_0) = \log(r^n) + \log(X_0) = n\log(r) + \log(X_0)$



4 A more complex model

Definition

Include some more realistic features:

- Immigration from mainland A
- Maximum population size / Carrying capacity K
- Mating more difficult in small populations: growth rate slow for small population size

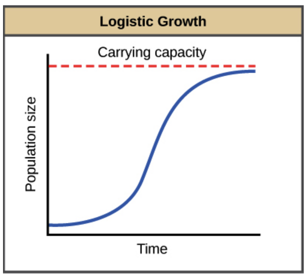


Image credit: "Environmental limits to population growth: Figure 1," by OpenStax College, Biology, CC BY 4.0.

5 Equilibrium and stability

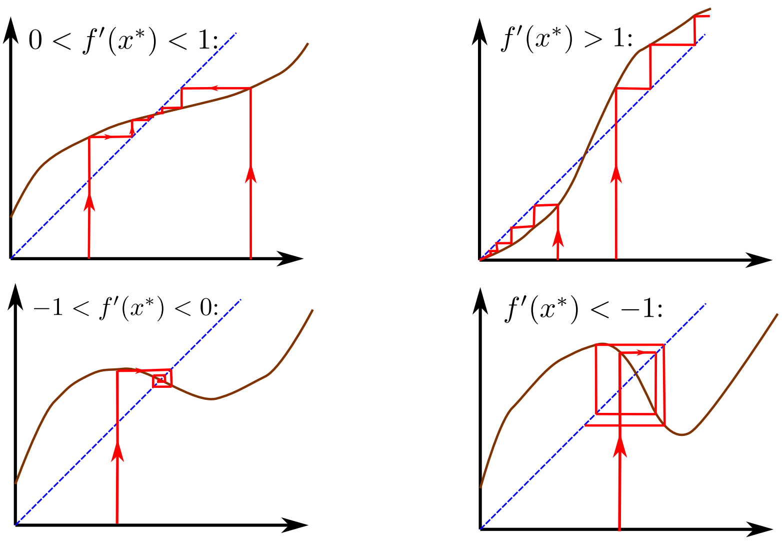
Long-term behaviour and fixed points

What is the state of the system on the long run?
Find $x^* = \lim_{n\to\infty} X_n$.

Candidates: Fixed points = points with $f(x) = x$ also called equilibrium points
If x^* is a fixed point and $X_n = x^*$ then $X_{n+1} = x^*$
Stability:

- x^* globally stable: $\lim_{n\to\infty} X_n = x^*$ for all X_0
- x^* locally stable: $\lim_{n\to\infty} X_n = x^*$ if X_0 close to x^*
- x^* unstable: not even locally stable

Stability of fixed points: the cobwebbing method



Stability of fixed points: the cobwebbing method

Draw the plot of $f(x)$ and add the line $y = x$.

- Start with X_0
- Go vertically to the curve: you find $f(X_0) = X_1$.
- Move horizontally to the $y = x$ line and then back vertically to the x-axis to have X_1 on the x-axis.
- Go vertically to the curve: you find $f(X_1) = X_2$.
- Move horizontally to the $y = x$ line and then back vertically to the x-axis.
- etc ...

See if you come closer to the fixed point or if you get away from it.
Repeat for several X_0.

Conclusion from examples drawn on the board:

- If $| f'(x^*) | < 1 \Rightarrow x^*$ is (locally) stable
- If $| f'(x^*) | > 1 \Rightarrow x^*$ is unstable

Reminder: derivation

Definition:

$$\tfrac{d}{dx} f(x) = f'(x) = \lim_{h \to 0} \tfrac{f(x+h)-f(x)}{h}$$

Examples:

$\tfrac{d}{dx} x^n = n \cdot x^{n-1}$
$\tfrac{d}{dx} e^x = e^x$
$\tfrac{d}{dx} \ln(x) = \tfrac{1}{x}$
$\tfrac{d}{dx} \cos(x) = -\sin(x)$
$\tfrac{d}{dx} \sin(x) = \cos(x)$

Derivation: rules

Linearity of differentiation

$$\begin{aligned} \frac{d}{dx}[f(x) + g(x)] &= f'(x) + g'(x) \\ \frac{d}{dx}[a \cdot f(x)] &= a \cdot f'(x) \end{aligned}$$

Product rule

$$\frac{d}{dx}[f(x) \cdot g(x)] = f'(x) \cdot g(x) + f(x) \cdot g'(x)$$

Quotient rule

$$\frac{d}{dx} \frac{f(x)}{g(x)} = \frac{f'(x) \cdot g(x) - f(x) \cdot g'(x)}{g(x)^2}$$

Chain rule

$$\frac{d}{dx} f(g(x)) = f'(g(x)) \cdot g'(x)$$

Reminder: integration

Definition:

$$F \text{ is the antiderivative of } f \text{ if and only if } F'(x) = f(x) \text{ and thus } F(x) = \int_c^x f(x)dx$$

We also have: $\int_a^b f(x)dx = F(b) - F(a) = F(x)\Big|_a^b$

Important antiderivatives:

$$\begin{aligned} f(x) = x^n \quad &\Rightarrow \quad F(x) = \frac{x^{n+1}}{n+1} + c \\ f(x) = \frac{1}{x} \quad &\Rightarrow \quad F(x) = \ln(x) + c \\ f(x) = e^{ax} \quad &\Rightarrow \quad F(x) = \frac{1}{a} e^{ax} + c \end{aligned}$$

6 The Verhulst model

Evolution of a bacterial population

Consider a population of bacteria in a medium:
If you have initially a small quantity of bacteria they will grow almost geometrically, but when the medium (or some essential elements in it) becomes rare their growth will slow down.

We make the following assumptions:

- no migration
- no small-population effect
- limited carrying capacity

Then the population size can be modelled by:
$X_{n+1} = X_n \cdot r(X_n) = X_n \cdot r_0 \frac{c}{c+r_0 X_n}$ with $r_0 > 0$ and $c > 0$
The reproduction rule is:
$f(x) = x \cdot r_0 \cdot \frac{c}{c+r_0 x}$

Asymptotics and derivatives

$$f(x) = \frac{x \cdot r_0 \cdot c}{c + r_0 \cdot x} = \frac{r_0 \cdot x}{1 + r_0 \cdot \frac{x}{c}} = \frac{r_0}{\frac{1}{x} + \frac{r_0}{c}}$$

Asymptotics:
$\lim_{x \to \infty} f(x) = \frac{r_0}{\frac{1}{\infty} + \frac{r_0}{c}} = \frac{1}{\frac{1}{c}} = c$

Derivatives:
$f'(x) = \frac{(c+r_0 x) \cdot r_0 c - x r_0 c r_0}{(c+r_0 x)^2} = \frac{c^2 r_0}{(c+r_0 x)^2} > 0$

$f'(0) = r_0$ initial growth rate

$f''(x) = \frac{(c+r_0 x)^2 \cdot 0 - c^2 r_0 2 (c+r_0 x) r_0}{(c+r_0 x)^4} = \frac{-2 \cdot c^2 r_0^2}{(c+r_0 x)^3} < 0 \to$ slowing down

Fixed points equation

$x = f(x) = \frac{x r_0 c}{c+r_0 x}$
$\Leftrightarrow (c + r_0 x) \cdot x = x r_0 c$
$x_1 = 0$
and for $x \neq 0$
$c + r_0 x_2 = r_0 c$
$\Leftrightarrow x_2 = \frac{r_0 c - c}{r_0} = c - \frac{c}{r_0}$

Case $r_0 \leq 1 \Rightarrow x_2 = c - \frac{c}{r_0} \leq 0 \to$ the only fixed point is $x_1 = 0$
Case $r_0 > 1 \Rightarrow x_2 = c - \frac{c}{r_0} > 0$:

$$f'(x_2) = \frac{c^2 r_0}{(c + r_0 x_2)^2} = \frac{c^2 r_0}{\left(c + r_0 \cdot \left(c - \frac{c}{r_0}\right)\right)^2} = \frac{c^2 r_0}{(c + r_0 \cdot c - c)^2} = \frac{c^2 r_0}{(r_0 \cdot c)^2} = \frac{1}{r_0} < 1$$

$\to$ fixed point x_2 is stable.

Some conclusions on the Verhulst model

- The Verhulst model can be used to describe the dynamics of the size of a bacterial population.
- Its long-term behavior depends on the initial growth rate parameter r_0.

Reminder: Soving linear or quadratic equations
Examples:

- $2 \cdot x + 6 = 12 \Leftrightarrow x = 3$
- $x^2 = -1 \Leftrightarrow x = \pm i$ (imaginary number)

Second degree equations:
$a \cdot x^2 + b \cdot x + c = 0$
Determinant Δ:
$\Delta = b^2 - 4 \cdot a \cdot c$

- if $\Delta < 0 \rightarrow$ no solution in $\mathbb{R}$
- if $\Delta = 0 \rightarrow$ unique solution $x = \frac{-b}{2 \cdot a}$
- if $\Delta > 0 \rightarrow$ two solutions $x = \frac{-b \pm \sqrt{\Delta}}{2 \cdot a}$

"Midnight formula":

$$\begin{aligned} 0 &= ax^2 + bx + c \\ \Rightarrow x_{1,2} &= \frac{-b \pm \sqrt{b^2 - 4 \cdot a \cdot c}}{2 \cdot a} \end{aligned}$$

"p q formula":

$$\begin{aligned} 0 &= x^2 + px + q \\ \Rightarrow x_{1,2} &= -\frac{p}{2} \pm \sqrt{\left(\frac{p}{2}\right)^2 - q} \end{aligned}$$

7 Transformation to a linear process

Consider 2 competing populations
The Verhulst model is not linear process whereas the geometric growth was $(f(x) = r \cdot x_n)$.
Now consider two populations competing for the same ressource so that they have the same growth limitation parameter c and their competition terms depend on the size of both populations:

- $a_{n+1} = a_n \cdot r_a \frac{c}{c + r_a a_n + r_b b_n} = f_1(a_n, b_n)$
- $b_{n+1} = b_n \cdot r_b \frac{c}{c + r_a a_n + r_b b_n} = f_2(a_n, b_n)$

The process is multi-dimensional and non-linear.

Consider the ratio of population sizes
Lets consider the ratio of the population sizes:
$Z_n = \frac{a_n}{b_n}$
$Z_{n+1} = \frac{a_{n+1}}{b_{n+1}} = \frac{a_n \cdot r_a}{b_n \cdot r_b} = Z_n \cdot \frac{r_a}{r_b} \rightarrow$ linear!

- Z_n grows exponentially for $r_a > r_b$
- Z_n shrinks exponentially for $r_a < r_b$
- $Z_n = Z_0$ for $r_a = r_b$

Some of the things you should be able to explain

- The different purposes of mathematical models in biology
- The meaning of the parameters in discrete-time models like the Verhulst model
- How to study fixed points and their stability for discrete-time models

  - By cobwebbing
  - Mathematically with derivatives

- The meaning of derivatives and how to calculate them
- How to solve quadratic equations and other simple equations.
- The trick to transform parameters to obtain a simpler process, e.g. a linear process