Week 1: What is Mathematical Biology?

Part of the `mathbio-primer` series of notes by theajs87

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Welcome to the mathematical biology primer course! My goal with this course is to provide an overview of the necessary mathematical tools you will need to start tackling quantitative biology research on your own. We'll start off nice and slow, by understanding what it is that we aim to achieve, and then build up to what we will be studying next week.

So... what is it?

Mathematical biology means something along the lines of "**using applied mathematics tools to represent and model biological systems**". That was quite self-explanatory, right? However, I'd say that there's slightly more to it than that. There are two main ways of viewing it:

- Focusing on the **biology** and using mathematics as a tool. This is what most people generally understand by the term, and is what we will be doing in this course.
- Focusing on the **mathematics**, and developing new techniques based off of the biology.

The former definition is what most people generally understand by the term 'mathematical biology', and is what we will be doing in this course. If you are interested in the latter way of thinking, it might still be useful for you to go through this course - feel free to skip ahead and see if this resource is helpful!

1 Course Content

There are many fields of applied mathematics (and sometimes even pure!) which are useful and applicable to theoretical biology. Here are the ones which I think are most relevant (and thus the ones we will be covering):

- **Dynamical Systems [weeks 2-4]**: This is the most accessible field with the least amount of prerequisite knowledge required. Broadly speaking, it is the study of **time-dependent systems**, hence 'dynamical'. In this course, we will specifically be looking at systems of ordinary differential equations (ODEs), and qualitatively analysing them. A (regrettably) very common example of where this is used is in modelling **population dynamics**.
- **Partial Differential Equations (PDEs) [week 5]**: The meaner counterpart to ODEs, PDEs also take into account a **spatial dependence** of the dynamics. **Pattern formation in nature** is usually the classic example for an application of this field. This is specifically the study of **reaction-diffusion systems** and **Turing instabilities**.
- **Stochastic Processes [week 6]**: In actual biological systems, there is a considerable amount of 'stochasticity' (noise) in everything that happens. Studying 'deterministic' (without randomness) models simplifies the analysis drastically, but completely ignores this very important factor. We can reintroduce this biological **noise** into our models via this field. For example, **stochastic modelling of reaction kinetics** is a fundamental application of this theory.
- **Graph Theory and Networks [week 7]**: A lot of biological networks can be modelled using the mathematical object known as a **graph**. For example, **protein-protein interaction networks, and transcriptional regulatory networks** can be represented in this way. This naturally means that concepts from graph theory are very easily applicable to these networks, e.g. **clustering** and **centrality measures**.

- **Bayesian Inference** [**week 8**]: By now, we've constructed lots and lots of models, but with no grounding in reality. Given real-world data, how do we make sure the model lines up with reality? We can use Bayesian inference to **estimate model parameters**.

In **weeks 9 & 10**, we will attempt to tie these concepts together and see what contemporary quantitative biology research looks like, and finish on AI & ML because... buzzwords.

2 Learning Objective

The goal with this course is not to get you to completely master all of these tools - it took me 3 years to be half-decent at them! Rather, the hope is that you will **feel comfortable with the basic terminology and concepts involved with each field**, so that you're not completely lost when trying to understand research papers in quantitative biology fields. It's a 'primer' course after all!

3 Ordinary Differential Equations (ODEs)

For this section, I assume that you know mathematical notation, and can differentiate and integrate. If not, don't worry - consult the calculus refresher, or your old secondary school textbooks!

3.1 What is a differential equation?

So, I hear you ask, what is a 'differential equation'? Put simply, a differential equation is **an equation that relates an unknown function to its derivatives**. For example, for some function $f(x)$ and some constant $\lambda \in \mathbb{R}$,

$$f'(x) = \lambda f(x)$$

is a differential equation.

- An **ordinary differential equation (ODE)** is a differential equation dependent on only one independent variable. In most applications, this variable would be the time t, i.e. the ODE would only consist of $t, f(t), f'(t), f''(t), \ldots$ – this simplifies things considerably!
- A **partial differential equation (PDE)** is a differential equation dependent on more than one independent variable. In the examples we'll see, these are usually space (x) and time (t) variables. More on that in week 5!

To start off, we'll only consider **scalar** functions $f : \mathbb{R} \to \mathbb{R}$ for simplicity. A general form for an ODE of **order** k is

$$G\left(x, f(x), \frac{\mathrm{d}f}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}^k f}{\mathrm{d}x^k}\right) = 0.$$

That is, the highest derivative present in the equation G is of order k. The **degree** of the ODE is the power of the highest derivative (when fractional powers have been removed). The ODE is **linear** if G is a linear function of $f(x)$ and its derivatives. This form of the ODE is the **implicit** form; the **explicit** form would have the highest order derivative as a function of the lower ones, i.e.

$$\frac{\mathrm{d}^k f}{\mathrm{d}x^k} = F\left(x, f(x), \frac{\mathrm{d}f}{\mathrm{d}x}, \ldots, \frac{\mathrm{d}^{k-1} f}{\mathrm{d}x^{k-1}}\right) = 0.$$

Example 3.1: ODE Terminology

Consider the following ODE for the function $f(x)$:

$$\frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = 5\left[1 + \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)^2\right]^{\frac{1}{3}}$$

This is a **non-linear**, **explicit** ODE of **degree** 3 and **order** 2.

3.2 Initial Value Problems, Existence and Uniqueness of Solutions

Consider the ODE

$$f'(x) = 3f(x).$$

$f(x) = e^{3x}$ is a solution, $f(x) = e^{3x} + 4$ is another, $f(x) = 420e^{3x}$ is yet another one. In fact, there are infinitely many solutions! It is then easy to see that simply considering ODEs on their own will get us nowhere; we need to choose which solution we want to look at. For that, we turn to initial value problems (IVPs).

Definition 3.1: Initial Value Problem (IVP)

An initial value problem is a differential equation along with an appropriate number (the order of the ODE) of **initial conditions** (the initial value of a differential equation).

In these first couple of weeks, we will consider biological systems that can be modelled as a one-dimensional or first-order system, i.e. IVPs of the form

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= f(x) \\ x(0) &= x_0 \end{aligned}$$

where $x(t)$ is a (real-valued) function of time (t) and $f(x)$ is a nice (real-valued) function of x.
In constructing our biological models as IVPs, it is useful to know whether a) a solution exists, and b) is unique. As it turns out, we can guarantee this provided that $f(x)$ is sufficiently 'nice', according to the following theorem (which we will not prove):

Theorem 3.1: Existence and Uniqueness Theorem

Consider the IVP

$$\begin{aligned} \frac{\mathrm{d}x}{\mathrm{d}t} &= f(x), \\ x(0) &= x_0. \end{aligned}$$

Suppose that $f(x), f'(x)$ are continuous on an open interval of the x-axis ($\mathbb{R}$), and suppose that x_0 is a point in $\mathbb{R}$. Then, the IVP has a solution $x(t)$ on some time interval $(-\tau, \tau)$ about $t = 0$, and the solution is unique.

For the majority of our modelling efforts, $f(x), f'(x)$ will be 'nice' enough for this theorem to hold, and so we won't have to worry about it. However, it is also important to note that it only applies over some interval $(-\tau, \tau)$ and not necessarily for all time.

Next week, we will have a look at how we can analyse these systems without explicitly solving them.