APPLIED MATHEMATICS AND MODELING

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ABSTRACT

Cast your mind back to school physics or chemistry and you're likely to recall a certain amount of mathematics involved. Boyle's law (relating pressure and volume of a gas), the law of gravity, Newton's second law (relating force, mass, and acceleration) — all mathematical formalisms of laws underpinning the world around us.

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These are mathematical models based on theories; if the maths doesn't match reality, it indicates the underlying theory may not be complete. These theorems are significant and underpin many of the advancements in engineering that enable our modern lives. However, much of the natural world is messier, more random, and more complex than systems to which laws can be applied.

Instead, mathematical modelling aims to break down complex systems into their key dynamics and interactions. These system features (say, the R rate…) are set out in mathematical form, with each term of the model equation representing a particular feature (usually, though not always the case). Isolating each feature as part of the wider model enables us to experiment with the system computationally, to determine which dynamics are most significant, and explore what impact any changes may have on the system, beyond the limitations of testing in real-life.These systems occur most frequently in biology, but the following discussion of the steps to build a successful mathematical model can be applied elsewhere in epidemiology, finance, weather forecasting, and managing systems such as agriculture and healthcare. Mathematical modelling offers unparalleled insight into how to predict, control, and optimise systems, that has become a fundamental part of how we interact with the natural world. The first step is to break a complex system down into the main features and interactions involved. Information about different parts of the system is drawn together from scientific literature, and specifically designed observation/experiments required to fill in any knowledge gaps, as we will see later. This puts together enough information for a conceptual model, sufficient to draw a diagram of what's going on, but not enough

information to make predictions about the system with any certainty. If we want to model the amount of morphogen at a particular point and time, we would likely include the following features:

- production of the morphogen, by a specific cell type;
- diffusion of the morphogen (spreading out into the surrounding area, like perfume droplets in the air);
- uptake (absorption) of the morphogen by other cell types, and
- degradation of the morphogen (i.e., they have a shelf-life, usually short in the unideal storage conditions of the body).

Further dynamics, such as the proliferation (cell division) of the cells responsible for morphogen production and uptake, cell death, and cell migration could also be considered. Deciding which features are necessary to include require consideration of the time and spatial scale you are interested in for the purpose of your model. Biology in particular works across vast scales; from gene dynamics inside the nucleus, to morphogen production and other cell-cell interactions, to tissue-level dynamics of a whole organ or the mechanics of a joint in the skeleton. Dynamics working across these different time and spatial scales will hold varying importance in a particular model, and may not need to be explicitly considered depending on the level of detail required. For example, production of a morphogen begins with DNA transcription in the cell's nucleus, with a flurry of other activity responsible for the secretion of each morphogen molecule by the cell. However, if we are on a tissue level, in which thousands of these molecules can be found per square area, we do not need to model the discrete number of molecules, and can instead model the concentration (a continuous variable). Similarly, if our timescale spans minutes or hours, rather than seconds or milliseconds, we will not need to explicitly consider what is happening inside each cell. Internal cell processes happen on such a comparatively fast scale that only the end result of the internal production dynamics is needed — the overall rate of production, rather than rate of transcription, etc. For this, we have the culmination of great minds turning their attention to the applications of mathematics to thank. A typical equation of a mathematical model today is, roughly speaking, formed of several terms that are each models in their own right. Each of our morphogen model features are a mini-system that have previously been researched and modelled. Diffusion models are tested and confirmed by experiments using dye in water; the model of production of a chemical by a cell is a result of many experiments over the years, that has shown us the dependence of such a model on both the type of chemical, cell type, and potentially the environment around it; the uptake of chemicals by cells is a similarly involved process.

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