Chapter 3: A career in modelling

Lecture 5: Learning how to model

Learning objectives

✓ Understand the framework for mathematical models in science

✓ Appreciate the uses and limitations of models

✓ Contrast data driven models with theoretically driven models

Scientific examples

✓ Blood flow through a bypass vein graft

Maths skills

✓ Understand and interpret data from a graph

In this chapter we discuss what mathematical modelling means in science, as well as different ways in which models are developed and understood. When developing models in science, there will always be a balance between theory and data driven models. We will cover a framework that discusses the differences between the two approaches, and note that they are often interlinked.

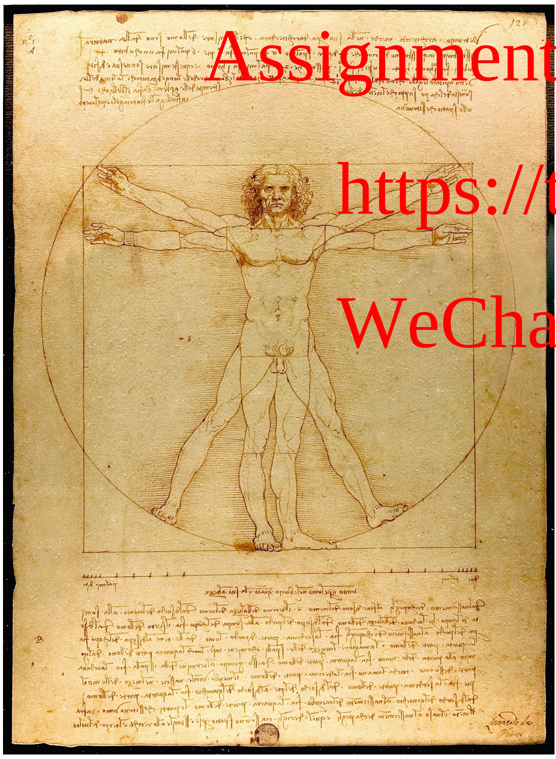

Image 3.1: *Vitruvian Man* (1490), Leonardo da Vinci. (Source: en.wikipedia.org)

We will practice the skill of developing a theoretical mathematical model in the context of blood flow through a blood vessel, and what this means for angioplasty procedures. We will also consider the results of a long-term study which uses large amounts of data to model the risk of coronary heart disease.

3.1 Intro to philosophy of models in science

Science

Science aims to **understand**, **explain**, **predict** and **influence** phenomena. Understanding science, and thinking in a 'scientific manner', requires:

- *discipline knowledge and content* – the language, information, knowledge and skills specific to a discipline; Not SCIE1000
- *scientific thinking and logic* – the conceptual process of performing systematic investigations, hypothesising, thinking critically and defensibly, and making valid deductions and inferences; SCIE1000!
- *communication and collaboration* – the process of working with others, sharing information and resources; SCIE1000!
- *curiosity, creativity and persistence* – the relatively intangible characteristics that underline the ability to ask and answer 'interesting' questions, and solve difficult problems in novel ways; BYO!
- *observation and data collection* – the processes and techniques used to collect useful data about particular phenomena; a little in SCIE1000
- *modelling and analysis* – the process of developing conceptual representations of phenomena, then using approximation, mathematics, statistics and computation in order to allow predictions to be made. lots in SCIE1000!

- Most science is intrinsically quantitative, because quantifying phenomena allows us to measure, describe and compare them efficiently and precisely.
- Science often proceeds by:
  - observing and measuring values, such as the amount, frequency, magnitude, duration or rate of some phenomenon; and
  - Using these data and scientific thinking to answer predictive questions about that phenomenon, such as
    - "What will happen if ...?"
    - "What causes ...?"
    - "How can ...?"
    - "Why does ...?"

Models

Models are simplifications and approximations of reality, usually based on measured data, that allow us to understand phenomena, make predictions and evaluate possible impacts of interventions. All models need to strike an appropriate balance between accuracy and complexity

- Models can be *physical* or *conceptual*. Examples of physical models include building scale models of bridges or dams, and subjecting the model to tests. In SCIE1000, we will focus on conceptual models.
- Ways of developing 'appropriate' models include:
  - using "common sense" and logical deduction;
  - using existing knowledge of similar phenomena; and
  - observing measured data and seeing what they "look like" (many phenomena change according to simple underlying patterns, such as at a constant rate or at a rate proportional to the current value).
- Some common ways of developing and presenting (conceptual) quantitative models are: words (descriptive text); values (for example, weight / height / age tables); pictures (such as graphs or flow diagrams); mathematics (using equations); and computer programs.
- Note that there is nothing "right" or "wrong" about each approach – each is suited to different uses and/or target audiences. See Appendix B for more information about communicating to a specific audience. Most models can be developed and presented in **all** of these ways.
- Scientists carefully examine the input and the output of a system in order to study and develop a deeper understanding of the system. If a system is well understood and there is a desired output, one may then control the input into the system in order to obtain that output (for example, in agriculture). If a system is understood and the input is known, then one may predict the output of that system; these predictions may cause some controversy, and the goal of a scientist is to refine and improve

the understanding of systems in order to make better, more accurate predictions.

$$\text{Input} \quad \rightarrow \quad \text{System} \quad \rightarrow \quad \text{Output}$$

- We will refer to this concept as the ISO (Input, System, Output) view of models. Knowing any two of the three provides one with the opportunity to understand the third.

- There are also two types of ways in which models are derived. We will consider both of these in SCIE1000.

Mechanistic Models vs Phenomenological Models

A **mechanistic model** is a model that is derived theoretically by examining the individual physical components of a system.

A **phenomenological model** is a model that is derived empirically by fitting a hypothesised relationship to the observed data.

- When developing a mechanistic model, it is important to ask yourself what are the key factors that could influence the phenomenon in question.

- Phenomenological models are usually determined using statistical software. In SCIE1000, you will not be required to run such software; instead we will discuss the basic features of mathematical functions that can be used to fit various sets of observed data. In this course, *critical thinking* will be valued more than precision.

- Mathematics provides a range of logically valid techniques that allow us to deduce information that we cannot measure or obtain in other ways (due to physical, ethical or financial limitations).

Question 3.1.1

For the following models, seen in earlier lectures, determine whether they were mechanistic or phenomenological models. Explain.

(a) The model for blood alcohol concentration we developed in Lecture 1.

Mechanistic – no data involved, just used modelling, common sense, thinking

$B = \frac{n}{m} - t$

(b) The Widmark formula for blood alcohol concentration we described in Lecture 2.

$B = \frac{A}{rm} \times 100\% - 0.015t$

Phenomenological – used data

(bit of both)

Question 3.1.2

Suppose a model has been developed phenomenologically with no underlying mechanism to explain it. Should you use the model to make predictions by extrapolating it? Why or why not?

Can we – yes!

Should we – maybe – only with caution

3.2 Mathematics and models

- Some people view mathematics as being an abstract process, unlike disciplines such as biology or chemistry that relate directly to the 'real' world. This view ignores the many links between mathematics and science:
  - Scientists use discipline knowledge and a special language to describe nature and the real world (for example, biologists use taxonomic categories, anatomical descriptions and medical terminology).
  - Mathematicians also use discipline knowledge and a special language to describe nature and the real world (for example, exponential and linear functions all describe relationships between natural phenomena).

Mathematics

Mathematics is a standardised formal language, way of thinking and body of knowledge that allow us to:

- develop models to represent reality;
- increase our understanding of phenomena;
- perform correct logical deductions;
- communicate unambiguously; and
- draw conclusions and make predictions.

- Everyone needs to learn some mathematical language and thinking for their personal and professional lives, but to gain proficiency in science requires a higher level of mathematical knowledge and sophistication.
- SCIE1000 aims to develop skills in using mathematics, but we do not study mathematics for its own sake, or develop new mathematical knowledge; if you wish to do that, enrol in discipline-based mathematics courses.
- Instead, we study mathematics **solely** to understand and model the 'real' world. For example, *mathematical functions* are the formal descriptions of patterns in data, *derivatives* describe the change in a value at a point in time, and *integrals* describe behaviour over a period of time.

Question 3.2.1

The following graph shows the measured blood flow rate in coronary artery bypass vein grafts during a single heart beat, after a patient underwent coronary bypass surgery (see [47]). Data points have been joined by straight lines for clarity.

$= 0.5 \frac{mL}{s} \times 0.1\ s$

$= 0.05\ mL$

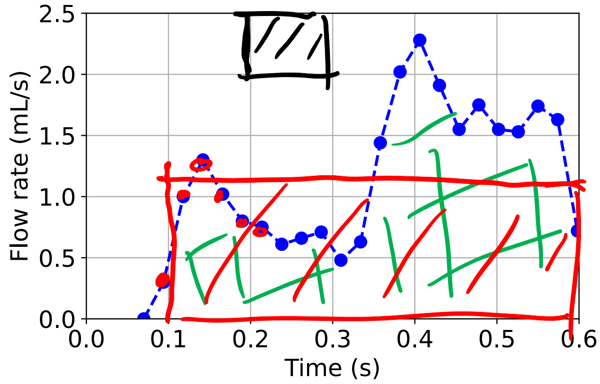

Figure 3.1: Blood flow rate in coronary artery bypass vein grafts, during a single heart beat.

Briefly discuss the physical meaning and significance of each of:

(a) The *height* or *value* of the graph at a given time.

Flow rate at a given time units mL/s

volume per unit time volume / time

(b) The *slope* or *rate of change* of the graph at a given time.

Change in the flow rate slope $= \frac{\text{rise}}{\text{run}}$

$\frac{mL/s}{s}$ => units mL/s^2

(c) The *area under the curve* of the graph over a time interval.

AUC = total volume during the time interval units mL

(d) Estimate the total blood flow through the vein graft in a heart beat.

height × width

$AUC = 1.2 \frac{mL}{s} \times 0.5\ s = 0.60\ mL$

Squares : 11 squares =>

$11 \times 0.05\ mL = 0.55\ mL$