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<u>Today</u>: "seminar" about math modelling.

<u>Wk 2</u>: Epidemics
<u>wk 3</u>: Pharmacokinetics (PK)

"Traditional" Maths Modelling:
Involves a lot of ODEs:

$$(1) \quad \frac{d\underline{x}}{dt} = \underline{V}(\underline{x}, t),$$

- $\underline{x}(t)$ is the state of the system;
- The "system" is described by some high-dimensional $\mathbb{R}^n$.
- The state of the system over time

is a trajectory in $\mathbb{R}^1$.

Models such as (1) are formulated via assumptions; these can rest on things like:

- Conservation laws
- Mass-action law

We try to use equations such as (1) for:

- Understanding
- Make predictions
- <u>Scenario Modelling</u>

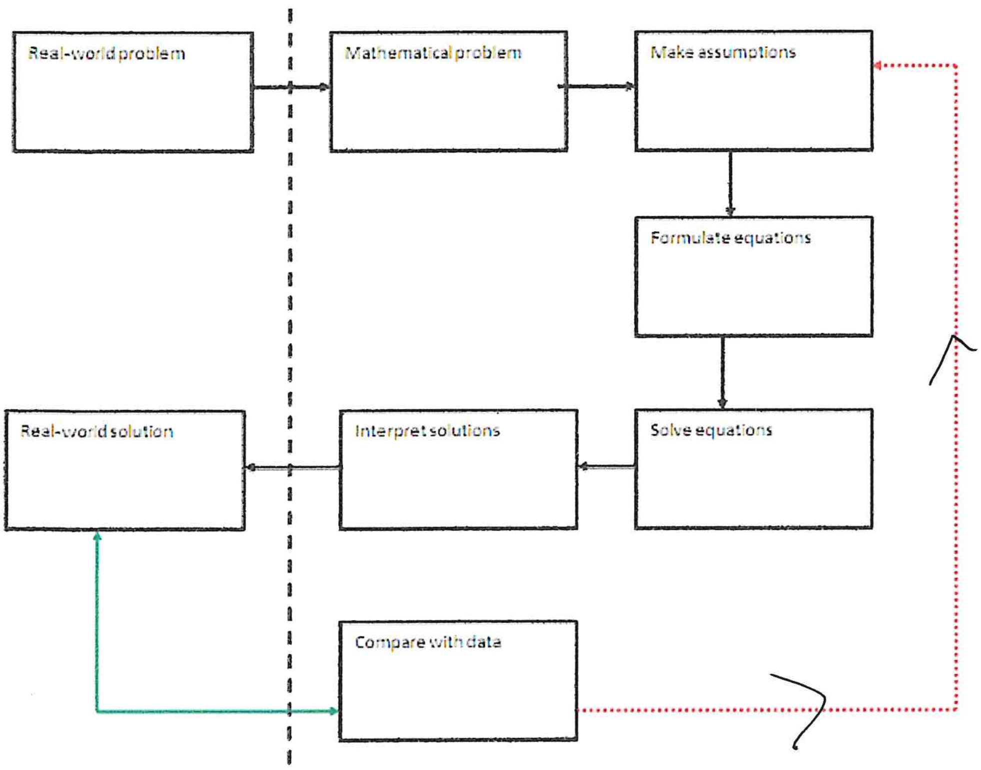


Figure 1.1: Flowchart showing the modelling process

1.1.1 Example

We look at a very basic example of how the modelling process in Figure 1.1 works. This is a bit of a silly, simplistic example, and it is important to note that the case studies and examples considered in the remainder of these lecture notes are much more detailed, realistic, and complex.

In any case, for the present purposes, consider the population of a fictitious country, Doriath. Let $P(t)$ be the number of people present at time t. We look at an exponential-growth model:

$$\boxed{P(t) = P(0)\mathrm{e}^{kt},} \tag{1.2}$$

where $P(0)$ is the population at time $t = 0$ and k is an unknown constant. Thus, to arrive back at the real-world solution, we need some data to determine k. For a problem involving time-evolution, this will be information about the past. For example, suppose we have the following data for the past fifty years (starting from $t = 0$). We overlay a curve of the kind (1.2) on the data (Figure 1.2) and choose a k-value that best fits the data. The result is $k = 0.021$. The result is not a perfect fit – it never will be. There will be small fluctuations in the population size for reasons unknown to this crude model. Nevertheless, the fit is good.

Suppose now we use the k-value to make a prediction for what the population will be in twenty

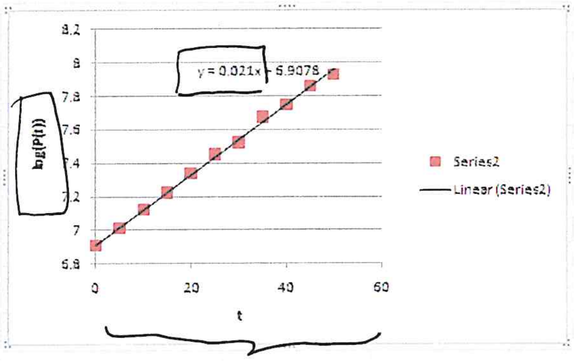
t (years)	P	t (years)	P
0	1000	30	1848
5	1110	25	2155
10	1239	40	2315
15	1372	25	2584
20	1540	50	2770
25	1727		

Table 1.1: Population of Doriath over fifty years.

t	P	ln(P)
0	1000	6.907755
5	1110	7.012176
10	1239	7.121864
15	1372	7.224274
20	1540	7.339552
25	1727	7.45386
30	1848	7.521826
35	2155	7.675739
40	2315	7.747037
45	2584	7.857107
50	2770	7.926483

$$P(t) = P(0)e^{kt}.$$

$$\boxed{\log(P(t))} = \log\left[P(0)e^{kt}\right] = k\boxed{t} + \log P(0).$$



$$k = 0.021.$$

Figure 1.2: Estimating the k-value from the data in Table 1.1.

years' time ($t = 70$):

$$P(t = 70) = 1000e^{0.021\times 70} = 4300 \text{ to two significant figures}$$

(our k-value has two significant figures, so we are only allowed to keep two here).

- If, in twenty years' time, the population is close to $P = 4300$, then our model is validated, and we gain confidence in it (broken red line does not need to be followed in Figure 1.1).
- If, however, in twenty years' time, the population prediction is wildly different from $P = 4300$, then we need to revisit the model assumptions in Figure 1.1.

In any event, this example shows a typical (but not essential) property of a mathematical model:

> Often, a mathematical model contains free parameters that need to be estimated from data before predictions can be made.

Modelling — A word of Warning (Ch. 2)

Basics of population modelling:

- Assumptions:
  - Random fluctuations (epidemics)
  - No migration (closed population)
  - ~~No~~ Infinite carrying capacity
  - Homogeneous population — every individual has an equal chance of giving birth / dying in a given interval of time.
- Based on the assumptions, only two numbers affect the population growth:
  - Per-capita birth rate, $\beta(t)$
  - Per-capita death rate, $\alpha(t)$.

- Model encoding assumptions:
  - Rate of change of population $P(t)$ per unit time:

$$\frac{dP}{dt}.$$

  - Birth rate: βP.
  - Death rate: αP.
  - Using the assumptions / conservation law:

$$\frac{dP}{dt} = \beta P - \alpha P.$$

$$\Rightarrow \boxed{\frac{dP}{dt} = kP}$$

Separation of variables, etc.

$$P(t) = P(0)e^{kt}$$

Hence, the final form for the solution of the model (2.3) is

$$P(t) = P(0)e^{kt}. \tag{2.4}$$

Remarks:

- The model gives a way of predicting future populations, once the initial population $P(0)$ is known.
- However, it contains an **unknown parameter**, k.
- In practice, to determine k, we would find a historic **time series** of the population and fit a curve of the type (2.4) to the data. This would give us an estimate of k.
- We would then use that estimated value of k to predict future values of the population.

2.1.1 Model validation

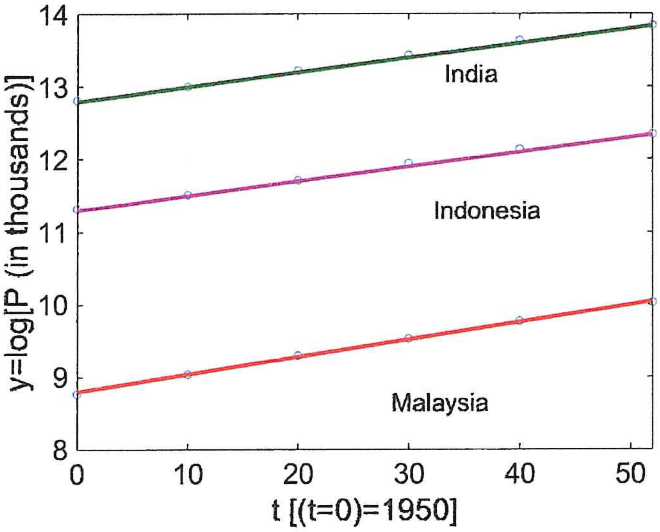


Figure 2.1: Census data and the Malthus model

The list of assumptions for the Malthus model does appear long. However, each one can be justified in detail. The things ruled out appear to be one-off events (epidemics and mass migration), and the model can therefore be expected to hold over long periods of time. The carrying capacity of the environment is large, so that again, resource limitations should not affect the population. Even the last point, concerning the sameness of the individuals in the population is not so unreasonable: there may be many atypical individuals in a society, but it is to be expected that there will be a sufficient mass of 'normal' individuals behaving in more-or-less the same way that the outliers can be ignored. Therefore, let us investigate a few human populations to see if they follow the model (2.4).

To validate the model (2.4) we are going to form the auxiliary quantity

$$y = \log(P),$$

such that, within the model,

$$y = kt + \log[P(0)].$$

If a population follows the model, its y-value, plotted against time, will be a straight line. It seems as though at least some populations do follow the Malthus model (Primary source: U.S. Census Bureau) – see Figure 2.1. However, let us look at China's population over the same period (Fig. 2.2). If the population were Malthusian, the 'line of best fit' would coincide with the actual data points.

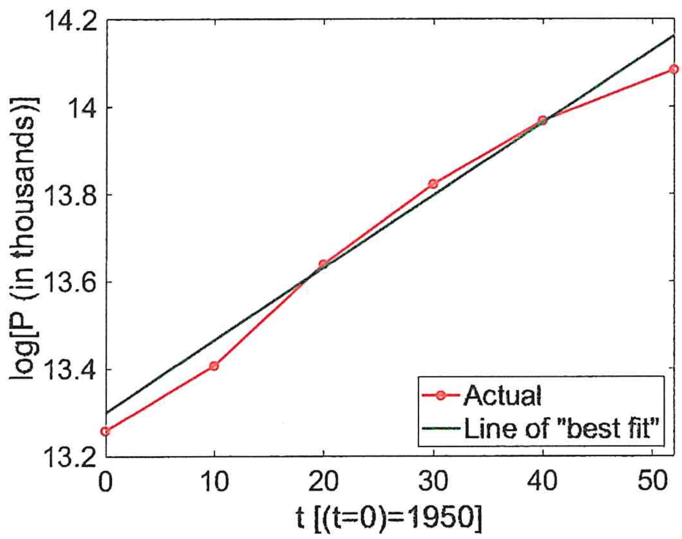


Figure 2.2: Census data for China and the Malthus model

However, the population deviates in a clear and systematic way from a straight line. The population here is not Malthusian.

It is salutary to try to discover where we have gone wrong in Figure 2.2. The dip in the first ten years of the graph could be due to the famine (1958-1961), while the dip in the latter years of the graph could be due to the one-child policy.

- The dip in the early years could be due to an increased death rate – larger α-value;
- The dip in the latter years could be due to a decreased birth rate – smaller β-value.

Both trends conspire to make k a function of time, such that the correct model would be

$$\frac{\mathrm{d}P}{\mathrm{d}t} = k(t)P, \qquad P(t) = P(0)\mathrm{e}^{\int_0^t k(t')\mathrm{d}t'}.$$

Word of warning — understand the limitations of modelling when it comes to <u>humans</u>. This is borne out by today's presentation, but also to the modelling of epidemics. Natural phenomena are easier to model than human populations!

Last words to Isaac Newton.

Successful theories:

- Laws of Motion
- Optics
- Fluid Mechanics
- Gravitation ...

Natural Phenomena

Newton could:

" calculate ~~of~~ the motions of the heavenly bodies, but not the madness of people".