CHEM2024 – Week 21 Lecture 2 – Building simple models

☐ *Sections 11.1-11.6 of Steiner, "The Chemistry Maths Book", 2nd edition.*

☐ *Sections 7.1-7.3 of Cockett and Doggett, "Maths for Chemists", Vol 1.*

1. Mathematical modelling of dynamic systems, early days

In Europe, the subject probably started with Fibonacci in 1202. He was looking at a rabbit population, for which he made the following assumptions: (a) each pair of rabbits reproduces once a month, producing another male-female pair; (b) each newly born rabbit pair takes a month to grow up; (c) rabbits never die. This model produces the following sequence for the number of rabbit pairs:

$$1,\ 1,\ 2,\ 3,\ 5,\ 8,\ldots \qquad i.e. \qquad x_{k+1}=x_k+x_{k-1} \tag{1}$$

This sequence became known as the *Fibonacci sequence*. It occurs in a variety of chemical and biological systems. However, as a rabbit population dynamics model, it is far from realistic.

In 1798 Malthus published his *Essay on the Principle of Population*. He assumed, that the birth count and the death count for humans are proportional to the headcount $x(t)$ at some point in the past:

$$x(t+\Delta t)=x(t)+ax(t)\Delta t-bx(t)\Delta t \tag{2}$$

where a is the birth rate and b is the death rate. Malthus recognised that, when food and space are plentiful, these parameters are constant. After rearranging and taking the limit, we obtain:

$$\frac{d}{dt}x(t)=\lim_{\Delta t\to 0}\frac{x(t+\Delta t)-x(t)}{\Delta t}=(a-b)x(t) \quad \Rightarrow \quad \frac{d}{dt}x(t)=\alpha x(t) \tag{3}$$

where $a-b=\alpha$ is called the *Malthusian coefficient* of the population. Significant approximations are involved in the derivation: the population count is assumed to be continuous and differentiable, the reproductive age is effectively zero, *etc.* But this model is a good start, and it works quite well at the initial stages of the population growth, when resources and space are both plentiful.

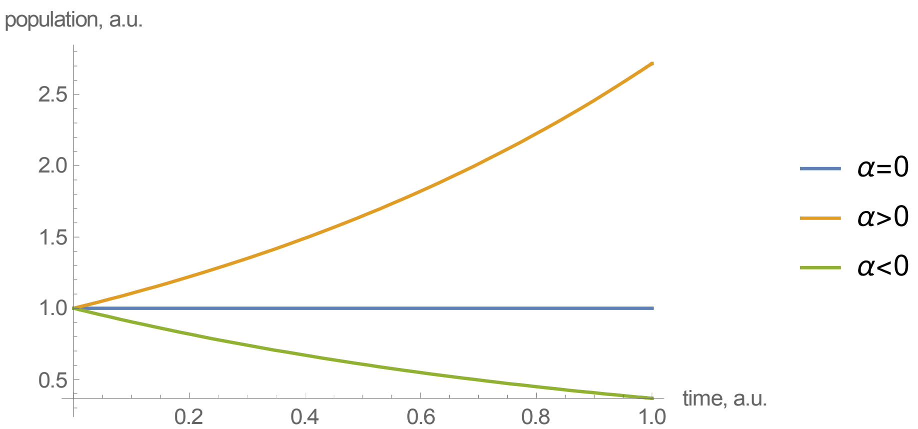

Figure 1. *Three regimes of the Malthus population model.*

Malthus was concerned about the fact that the steady state solution to his model was unstable (Figure 1). He saw from the census data that $\alpha>0$ for the UK population. That meant that, at some point, the population would run out of resources. Based on the history of his continent, he concluded that disasters – epidemics, wars, famines, *etc.* – were returning the population to a sustainable level.

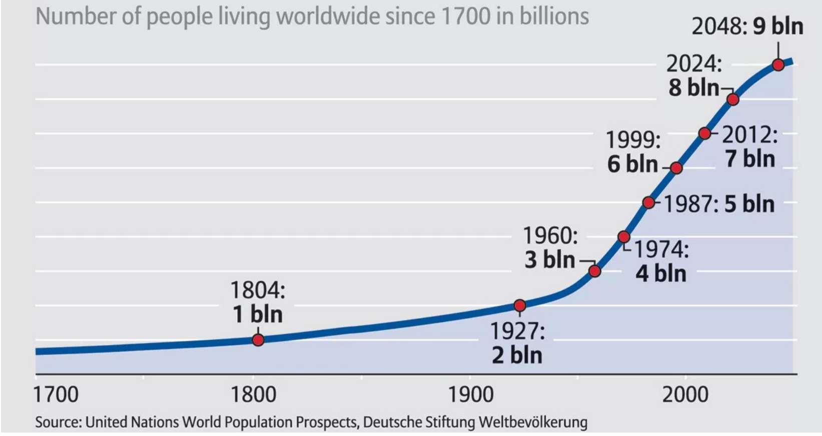

Figure 2. *Human population of the Earth in the last 300 years, and a forecast to 2048. Between 1700 and 1900, the exponential function was a very good approximation.*

The solution to the differential equation describing Malthus's model:

$$x(t) = x(0)e^{\alpha t} \tag{4}$$

was a good approximation to the real census data between 1700 and 1900 (Figure 2). This made Malthus's book influential and (as ever with honest biological and statistical research) heavily criticised by left-wing politicians and economists, most notably Karl Marx. The book was praised by Darwin and Wallace.

2. Continuous population models

Malthus model is a special case of a broader class of population models. Assuming a genderless population with a continuous and differentiable headcount, and no external influences, the equation describing the population dynamics would be:

$$x(t+\Delta t) = x(t) + B(x,\Delta t) - D(x,\Delta t) \tag{5}$$

where $B(x,\Delta t)$ is the birth count in the population of size x in a period Δt, and $D(x,\Delta t)$ is the death count. The following common sense conditions exist for the birth and the death counts:

$$\begin{cases} B(0,\Delta t) = 0 \\ B(x,0) = 0 \end{cases} \qquad \begin{cases} D(0,\Delta t) = 0 \\ D(x,0) = 0 \end{cases} \tag{6}$$

If the time increment Δt is small, both quantities may be approximated by the tangent lines:

$$\begin{gathered} B(x,\Delta t) \approx B(x,0) + b(x)\Delta t \\ D(x,\Delta t) \approx D(x,0) + d(x)\Delta t \end{gathered} \tag{7}$$

where $b(x)$ and $d(x)$ are the corresponding slopes. Equation (5) becomes:

$$\begin{gathered} x(t+\Delta t) = x(t) + b(x)\Delta t - d(x)\Delta t \\ b(0) = 0, \qquad d(0) = 0 \end{gathered} \tag{8}$$

Malthus had $b(x) = ax$ and $d(x) = bx$. In general, the limit of $\Delta t \to 0$ yields

$$\frac{dx}{dt} = b(x) - d(x) \tag{9}$$

3. Phase space analysis for autonomous ODEs

It is often necessary to analyse *every possible pattern of behaviour* in the solutions of autonomous ODEs such as the one in Equation (9). Plotting the time derivative of x against x produces a *phase space* plot that may be used to discover and interpret all dynamical modes of the system.

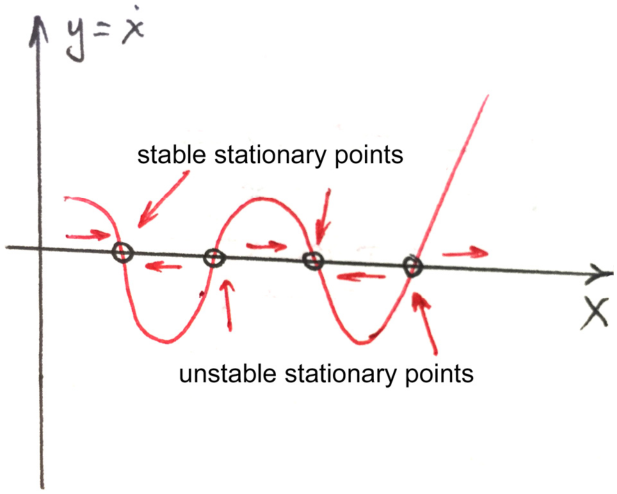

Figure 3. *An example of phase space analysis for an autonomous first-order ODE like the one in Equation (9). In the areas where the right hand side is positive, x(t) would grow with time; in the areas where the RHS is negative, it would decay.*

Figure 3 illustrates the concept of *phase space analysis* for autonomous first-order differential equations. The time derivative (or, equivalently, the right hand side) is plotted against the value of the unknown function $x(t)$. The plot shows where the system is going to move when it starts at any particular point.

Some points have zero derivative – the system does not move when it starts there. Those points are called *stationary points*. A *stable stationary point* is a steady state that restores itself when small perturbations are applied. An *unstable stationary point* is the one that does not.

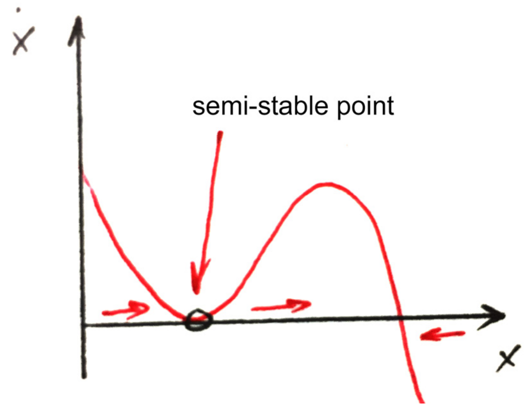

Figure 4. *An example of a semi-stable point, where the time derivative touches zero, but does not become negative.*

Semi-stable stationary points are those where the time derivative touches zero, but does not become negative. They are not significant in practice due to the uncertainties involved in the measurement of chemical and biological parameters.

The insight from Figure 3 leads to the formulation of the *stability condition* for stationary points for the population models of the type given in Equation (9):

$$\begin{cases} b(x) - d(x) = 0 \\ b'(x) - d'(x) < 0 \end{cases} \qquad (10)$$

We can therefore predict all dynamic regimes that can occur in the system. Depending on the initial condition and external influences, the system would drop into different stationary states.

3. Logistic model

An improvement of Malthus model was suggested in 1838 by Pierre-Francois Verhulst. He noted that the frequency of encounters between individuals in a population of size x is proportional to x^2, and that the encounters are the primary source of mortality due to fights, epidemics and other processes that reduce the headcount. He therefore suggested a modification to the Malthus model:

$$\frac{dx}{dt} = \alpha x - \beta x^2 \qquad (11)$$

where α is the Malthusian parameter and $\beta > 0$ is the *self-regulation coefficient*.

Phase space analysis for Equation (11) returns two stationary states (Figure 5): an unstable point when there's nobody at all in the population, and a stable point at $x = \alpha/\beta$. The parameter α/β is called *ecological niche capacity*.

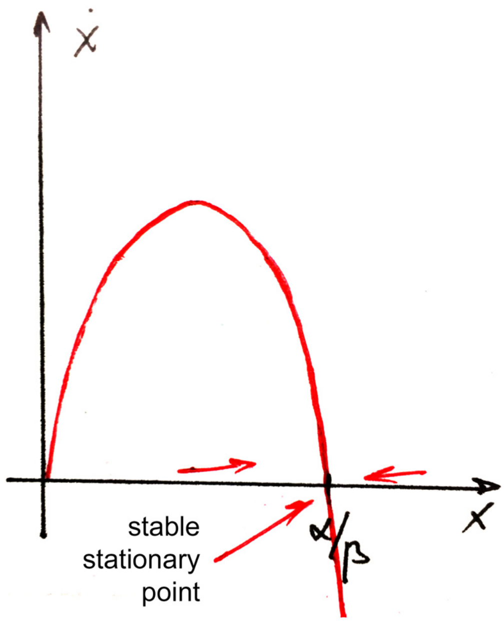

Figure 5. *Phase space analysis for Equation* (11).

Equation (11) is easily solved by variable separation:

$$\frac{dx}{\alpha x - \beta x^2} = dt \quad \Rightarrow \quad \alpha^{-1} \ln x - \alpha^{-1} \ln(\alpha - \beta x) = t + c$$

The initial condition is $x(0) = x_0$, and therefore:

$$x(t) = \frac{\alpha x_0 e^{\alpha t}}{\alpha - \beta x_0 + \beta x_0 e^{\alpha t}} \qquad (12)$$

The corresponding curve is called *logistic curve*. Three examples of solutions are shown in Figure 6.

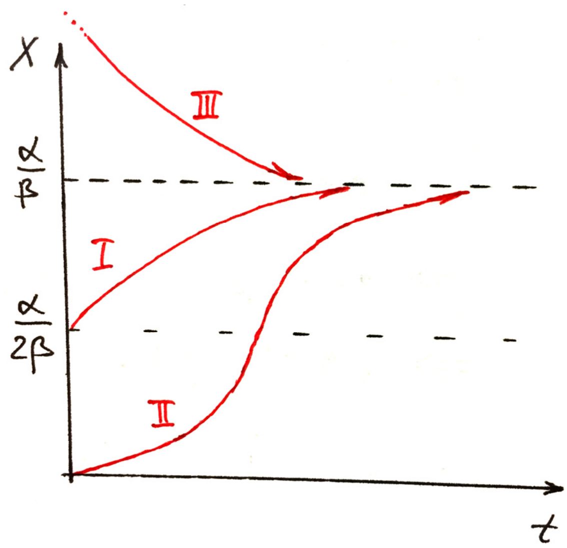

Figure 6. *Schematic drawings of some limiting case solutions of the logistic model.*

Solution (I) starts with a significant population that is below the niche capacity. The headcount grows monotonically and asymptotically approaches the capacity. Solution (II) is when the initial population is non-zero, but far below the niche capacity – note the similarity to Figure 2; the initial behaviour is Malthusian. Solution (III) starts at the headcount that is above the niche capacity and asymptotically approaches it from above.