MARS

MATH4120

Mathematical Modelling and Programming

Lecture Notes

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Contents

Chapter 1

What is a mathematical model?

Learning outcomes

By the end of this week you should be able to:

- describe the modelling cycle and apply it to a simple real-world situation;
- identify the dimensions of physical quantities and check dimensional homogeneity;
- derive and solve a simple first-order ODE arising from a rate law;
- interpret the parameters of an exponential model in context.

1.1 The modelling cycle

Mathematical modelling is the process of translating a real-world phenomenon into the language of mathematics, analysing the result, and then translating back to make predictions or gain understanding.

Definition: Mathematical model

A **mathematical model** is a set of equations, together with assumptions and parameter values, that describes or approximates the behaviour of a real-world system.

No model is a perfect description of reality — and that is fine. A model is a tool, judged by whether it is *useful* for the question at hand. As the statistician George Box put it: *"All models are wrong, but some are useful."*

1.1.1 The modelling cycle

Building and using a model typically follows a cycle:

1. **Observe**: identify the phenomenon and the question you want to answer.
2. **Simplify**: make assumptions to reduce the problem to something tractable.
3. **Formulate**: express the assumptions as equations.
4. **Solve**: find solutions analytically or numerically.
5. **Interpret**: translate the mathematical output back into the real-world context.
6. **Validate**: compare predictions with data or known behaviour.

7. **Refine**: relax assumptions, add complexity, and repeat.

We will follow this cycle throughout the course, starting with very simple models and building up to richer ones.

1.2 Units and dimensional homogeneity

Every physical quantity has **dimensions** — the type of measurement it represents — and is expressed in particular **units**. The most common dimensions are:

Dimension	Symbol	SI unit
Length	L	metre (m)
Mass	M	kilogram (kg)
Time	T	second (s)
Temperature	Θ	kelvin (K)

We write $[Q]$ for the dimensions of a quantity Q. For example, $[\text{speed}] = L\,T^{-1}$, i.e. metres per second.

Key idea

Dimensional homogeneity: every term in a valid equation must have the same dimensions. You can use this as a quick sanity check on any formula.

Example Checking a formula

Newton's second law states $F = ma$. Check dimensional homogeneity.
$[F] = M\,L\,T^{-2}$ (force, in newtons), $[m] = M$, $[a] = L\,T^{-2}$. So $[ma] = M \cdot L\,T^{-2} = M\,L\,T^{-2}$. ✓

Exercise

The period of a simple pendulum of length ℓ in gravitational field g is claimed to be

$$T = 2\pi\sqrt{\frac{\ell}{g}}.$$

Check dimensional homogeneity. What are the dimensions of g?

1.3 A first model: exponential growth

1.3.1 Deriving the model from a rate law

Suppose a population of bacteria doubles every hour under ideal conditions. Let $N(t)$ denote the population size at time t (measured in hours).

The simplest assumption is that the *rate of change* of the population is proportional to the current population:

$$\frac{\mathrm{d}N}{\mathrm{d}t} = r\,N,$$

where $r > 0$ is the **growth rate** (units: per hour, i.e. $[r] = T^{-1}$). This is a **first-order ordinary differential equation (ODE)**.

1.3.2 Solving by separation of variables

Separate and integrate:

$$\frac{\mathrm{d}N}{N} = r\,\mathrm{d}t \implies \ln N = r\,t + C \implies N(t) = N_0\,e^{rt},$$

where $N_0 = N(0)$ is the initial population.

Example Bacterial growth

Suppose $N_0 = 100$ and the population doubles every hour, so $N(1) = 200$. Find r. From $200 = 100\,e^{r\cdot 1}$ we get $r = \ln 2 \approx 0.693$ per hour. The population at time t is $N(t) = 100\,e^{0.693\,t}$.

1.3.3 Interpreting the parameters

- N_0: the initial value — set the scale of the population.
- $r > 0$: exponential growth; $r < 0$: exponential decay; $r = 0$: constant.
- **Doubling time**: the time t_d such that $N(t_d) = 2N_0$ is $t_d = \ln 2/r$.
- **Half-life**: for decay ($r < 0$), the time to halve is $t_{1/2} = \ln 2/|r|$.

The same equation $\frac{\mathrm{d}N}{\mathrm{d}t} = rN$ models radioactive decay (with $r < 0$), continuously-compounded interest, and Newton's law of cooling (with a shift). This universality is one reason ODEs are so powerful.

Exercise

A radioactive isotope has a half-life of 5730 years (carbon-14).

(a) Find the decay rate r.

(b) What fraction of the original material remains after 1000 years?

(c) Write a sentence explaining what the sign of r means physically.

Exercise

A cup of coffee is at 90°C in a room at 20°C. Assume Newton's law of cooling:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -k(T - T_{\text{room}}), \quad k > 0.$$

Let $\theta = T - T_{\text{room}}$. Show that $\theta(t) = \theta_0\,e^{-kt}$ and hence $T(t) = T_{\text{room}} + (T_0 - T_{\text{room}})\,e^{-kt}$.

Chapter 2

Dimensional analysis and nondimensionalisation

Learning outcomes

By the end of this week you should be able to:

- identify characteristic scales in a physical problem;
- nondimensionalise a first-order ODE by introducing dimensionless variables;
- interpret the resulting dimensionless parameters;
- explain why nondimensional solutions are universal (solution collapse).

2.1 Characteristic scales

When we write down a model, the variables and parameters carry units. For instance, in Newton's cooling law

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -k(T - T_\infty),$$

the temperature T is in kelvin, t in seconds, k in s^{-1}, and T_∞ is a reference temperature.

A **characteristic scale** is a representative value of a quantity that captures the natural "size" of that quantity in the problem. Common choices:

- For temperature excess: $T_0 - T_\infty$, the initial excess above ambient.
- For time: $1/k$, the natural relaxation time.
- For length: the size of the domain or a physical feature.

The idea is to make variables dimensionless by dividing by their characteristic scale. This removes units and reduces the number of parameters.

2.2 Nondimensionalisation: the procedure

1. Identify all dimensional variables and parameters.
2. Choose a characteristic scale for each variable.
3. Define dimensionless variables by dividing by those scales.
4. Rewrite the equation in terms of the dimensionless variables.
5. Read off the dimensionless parameters that appear.

2.3 Worked example: Newton's cooling

Consider again

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -k(T - T_\infty), \qquad T(0) = T_0.$$

Step 1. Dimensional variables: T (temperature, K), t (time, s). Parameters: k [s^{-1}], T_∞ [K], T_0 [K].

Step 2. Characteristic scales: temperature scale $\Delta T = T_0 - T_\infty$, time scale $\tau = 1/k$.

Step 3. Define

$$\theta = \frac{T - T_\infty}{T_0 - T_\infty}, \qquad s = k\,t.$$

Both θ and s are dimensionless.

Step 4. Rewrite the ODE. Note $T = T_\infty + (T_0 - T_\infty)\theta$ and $t = s/k$, so

$$\frac{\mathrm{d}T}{\mathrm{d}t} = (T_0 - T_\infty)\,\frac{\mathrm{d}\theta}{\mathrm{d}s} \cdot k.$$

Substituting:

$$(T_0 - T_\infty)\,k\,\frac{\mathrm{d}\theta}{\mathrm{d}s} = -k\,(T_0 - T_\infty)\,\theta.$$

Step 5. Divide through:

$$\boxed{\frac{\mathrm{d}\theta}{\mathrm{d}s} = -\theta, \qquad \theta(0) = 1.}$$

This is a *universal* equation — it contains no parameters at all. Its solution is simply

$$\theta(s) = e^{-s}.$$

Key idea

By choosing the right scales, we have removed all parameters. *Every* Newton's cooling problem — regardless of k, T_0, T_∞ — maps to the same dimensionless solution $\theta = e^{-s}$. This is **solution collapse**.

2.4 Solution collapse

To visualise collapse: suppose you solve the dimensional problem for three different values of k (say 0.1, 0.5, and 2.0 s^{-1}) and plot $T(t)$ vs t. You get three distinct curves.

Now plot $\theta(s) = (T - T_\infty)/(T_0 - T_\infty)$ vs $s = kt$ for all three. All three curves coincide exactly on e^{-s}. This is the power of nondimensionalisation.

Example Logistic growth — nondimensionalisation preview

The logistic equation is

$$\frac{\mathrm{d}N}{\mathrm{d}t} = r\,N\left(1 - \frac{N}{K}\right), \qquad N(0) = N_0.$$

Let $u = N/K$ (dimensionless population) and $s = rt$ (dimensionless time). Show that

$$\frac{\mathrm{d}u}{\mathrm{d}s} = u(1 - u), \qquad u(0) = N_0/K.$$

The original three parameters (r, K, N_0) reduce to just one: N_0/K.

2.5 Dimensionless groups and physical meaning

When nondimensionalising a more complicated equation, not all parameters always cancel. What remains are **dimensionless groups** — combinations of the original parameters that have no units.

These groups carry physical meaning. For instance:

- The **Reynolds number** $Re = \rho U L/\mu$ in fluid mechanics compares inertial to viscous forces.
- The **Damköhler number** Da in chemistry compares reaction to diffusion timescales.

A single dimensionless group governs the qualitative behaviour of the solution. Next week we will see a systematic method — the Buckingham Π theorem — for finding these groups from the dimensional parameters alone.

Exercise

The equation for a damped pendulum is

$$mL^2\,\ddot{\theta} + bL^2\,\dot{\theta} + mgL\,\sin\theta = 0.$$

(a) Identify all dimensional quantities and their dimensions.

(b) Choose characteristic scales for angle and time.

(c) Show that nondimensionalisation leads to

$$\ddot{u} + \gamma\,\dot{u} + \sin u = 0,$$

where $\gamma = b/\sqrt{mgL/L^2}$ (or similar, depending on your choice of time scale) is the only dimensionless parameter. State clearly what γ measures physically.

Exercise

A chemical concentration C evolves as

$$\frac{\mathrm{d}C}{\mathrm{d}t} = -\frac{C}{\tau_r} + S,$$

where τ_r is a reaction timescale and S is a constant source.

(a) Nondimensionalise using $C^* = C/(S\tau_r)$ and $s = t/\tau_r$.

(b) What is the steady state of the nondimensional equation?

(c) What does this tell you about the original dimensional steady state?