Lecture slides

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Lecture 1

- Introduction to MA42002
- Conservation equations
- Examples of spatially homogeneous models

Conservation equations

$$\begin{pmatrix} \text{rate of change} \\ \text{in the population density} \end{pmatrix} = (\text{spatial movement}) + \begin{pmatrix} \text{birth, growth, death,} \\ \text{production or degradation} \\ \text{due to chemical reactions} \end{pmatrix}$$

Spatially homogeneous models (MA32009 revision)

Example problem - bacteria in a dish

$$N(t+\Delta t) = \quad N(t) + \quad KN(t)\Delta t.$$

A model for cell growth under nutrient depletion

$$\begin{aligned} \frac{dN}{dt} &= K(c)N = \kappa c N, \\ \frac{dc}{dt} &= -\alpha \frac{dN}{dt} = -\alpha \kappa c N, \end{aligned} \tag{1}$$

Leading to the logistic growth equation

The last equation can be rewritten as

$$\frac{dN}{dt} = \rho N \, (1 - \frac{N}{B}) \qquad\qquad N(0) = N_0, \tag{2}$$

Can also consider other biological processes

Exercise

Consider a well mixed bio reactor.

A biologist cultures an initial cell population of size N_0 in the bioreactor for 72 h.

Cells undergo division with a period of 14 h.

Each cell produces a non-degradable waste product, W, at rate k_1.

When total waste levels exceed a threshold, W^*, cell division stops. Otherwise the cell population grows exponentially.

How many cells are there at the end of the experiment?

Model development

Model checklist

1. Variables (dependent, indepedent ?)
2. Schematic diagram - what processes are being modelled?
3. Governing equations?
4. Define model parameters?
5. Initial conditions?

Exercise solution

Recap

- Is course layout clear
- Introduction to conservation equation
- Deriving spatially homogeneous models

Lecture 2

- Continue example
- Introduce SIR model
- Introduce an activator inhibitor model
- Derive a conservation equation

Exercise

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When total waste levels exceed a threshold, W^*, cell division stops. Otherwise the cell population grows exponentially.

How many cells are there at the end of the experiment?

The SIR model (used in Chapter 7)

Consider the SIR model equations:

$$\begin{aligned}\frac{dS}{dt} &= -rIS,\\ \frac{dI}{dt} &= rIS - aI,\\ \frac{dR}{dt} &= aI.\end{aligned}$$

What are the variables? What are the parameters?

Identify an expression for the reproduction number, R_0.

Hence explain why the condition $R_0 < 1$ is necessary to avoid an epidemic?

SIR model Calculations

$$\frac{dS}{dt} = -rIS,$$
$$\frac{dI}{dt} = rIS - aI,$$
$$\frac{dR}{dt} = aI.$$

An activator inhibitor model (used in Chapter 6)

Assume that species A is produced at constant rate k_1 and degrades at rate k_2.

Assume that B is produced at a constant rate, k_4.

Consider the reaction schematic

$$2A + B \rightarrow 3A,$$

with reaction rate k_3.

Write down governing ODEs.

Activator-inhibitor model

Consider the ODEs

$$\frac{da}{dt} = k_1 - k_2 a + k_3 a^2 b,$$
$$\frac{db}{dt} = k_4 - k_3 a^2 b,$$

Identify the steady state of the ODEs. How would you compute linear stability of the steady state?

Recap

- Introduced SIR and activator-inhibitor models
- Computed steady states and stability analysis

Lecture 3 Spatiotemporal models

- Derive conservation PDEs
- Consider different models of fluxes

Spatiotemporal models - derivation

Consider a spatial domain V. A conservation equation can be written either in terms of the mass or number of particles of a species as follows:

$$\begin{pmatrix} \text{rate of change of} \\ \text{number of particles} \\ \text{per unit time} \end{pmatrix} = \begin{pmatrix} \text{rate of entry of} \\ \text{particles into } V \\ \text{per unit time} \end{pmatrix} - \begin{pmatrix} \text{rate of exit of} \\ \text{particles from } V \\ \text{per unit time} \end{pmatrix}$$
$$+ \begin{pmatrix} \text{rate of degradation} \\ \text{or creation of particles} \\ \text{in } V \text{ per unit time} \end{pmatrix}$$

Deriving a conservation equation in 1D

$$\frac{\partial}{\partial t}\int_{x}^{x+\Delta x} c(\tilde{x},t)A d\tilde{x} = J(x,t)\,A - J(x+\Delta x,t)\,A + \int_{x}^{x+\Delta x} f(\tilde{x},t,c(\tilde{x},t))\,A\,d\tilde{x}. \tag{3}$$

A conservation PDE in 1D

$$\frac{\partial}{\partial t} c(x,t) = -\frac{\partial}{\partial x} J(x,t) + f(x,t,c(x,t)). \tag{4}$$

Generalising to R^n

$$\frac{\partial}{\partial t}\int_V c(x,t)\,dx = -\int_S J(x,t)\cdot\mathbf{n}\,d\sigma + \int_V f(x,t,c)dx.$$

Fluxes - Fickian diffusion

$$\mathbf{J} = -D\nabla c, \tag{5}$$

Fluxes - Nonlinear diffusion

$$D = D(c), \qquad \text{e.g. } D(c) = D_0 c^m, \quad D_0 > 0,$$

Hence

$$J = -D(c)\nabla c$$

Fluxes - Convection/advection

$$\mathbf{J} = \mathbf{v}c, \tag{6}$$

Fluxes - Taxis

$$\mathbf{J} = \chi(a)c\nabla a,$$

Domain of definition of the problem

Lecture 4

- Boundary and initial conditions
- Nondimensionalisation
- Model formulation

Boundary conditions

- Dirichlet
- Neumann
- Robin

Initial conditions

Formulating a model

Lecture 5

- Introduce a linear reaction diffusion model
- Diffusion

Linear reaction diffusion equation

$$\frac{\partial c}{\partial t} = D\nabla^2 c + f(c), \quad c \equiv c(\mathbf{x}, t), \;\; \mathbf{x} \in \mathbb{R}^n, \; t > 0.$$

so in 1D Cartesian coordinates

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + f(c), \quad x \in \mathbb{R}, \; t > 0.$$

1D diffusion equation with delta IC

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}, \quad x \in \mathbb{R},\ t > 0. \tag{7}$$

$$c(x_0, 0) = \delta_0(x) \qquad x \in \mathbb{R}, \tag{8}$$

where δ_0 is a *Dirac delta distribution* (Dirac measure) satisfying

$$\int_{-\infty}^{+\infty} \delta_0(x) = 1 \quad \text{and} \quad \int_{-\infty}^{+\infty} f(x)\delta_0(x) = f(0), \text{ for continuous } f.$$

Numerical solution

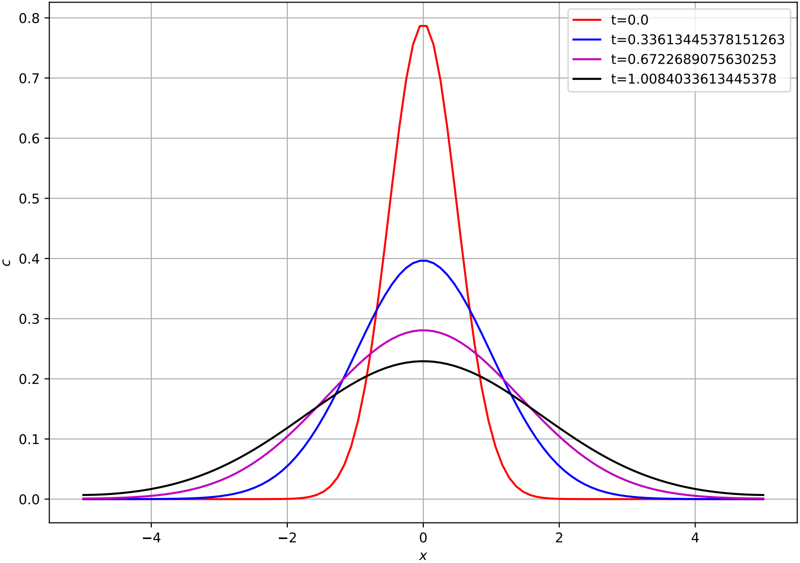

Figure 1: Numerical solution of diffusion equation.

An exact solution computed using a *similarity* variable

Consider the diffusion Equation 7 with initial condition Equation 8.

Introduce the similarity variable

$$\eta = \frac{x}{\sqrt{Dt}}$$

and look for solution of the form

$$c(x,t) = \frac{1}{\sqrt{Dt}} F(\eta).$$

Hence it can be shown that the explicit (analytic) solution is given by

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right). \tag{9}$$

The 1D diffusion equation for arbitrary initial condition

For a general initial condition $c(x, 0) = c_0(x)$ for $x \in \mathbb{R}$:

$$c(x,t) = \int_{-\infty}^{+\infty} \frac{c_0(y)}{\sqrt{4\pi D t}} \exp\left(-\frac{(x-y)^2}{4Dt}\right) dy.$$

Key properties of the (linear) diffusion equation (heat equation)

- The solution is infinitely smooth.
- The solution $c(x,t)$ stays positive for all $t > 0$ and $x \in \mathbb{R}$ if $c(x,0) > 0$ for $x \in \mathbb{R}$.
- The solution "propagates" with infinite speed i.e. for any $t > 0$, the solution is everywhere in $\mathbb{R}$.
- If we change the initial data $c(x,0)$ (continuously) then the solution also changes (continuously).

Diffusive transit time

$$D\frac{d^2c}{dx^2} = 0 \quad \text{in } (0, L), \quad c(0) = C_0,\, c(L) = 0.$$

Diffusion as a description of random walk

Suppose that the probability of a particle hopping distance Δx to the right in time Δt is

$$\lambda_R \Delta t.$$

Similarly, the probability of hopping a distance Δx to the left is

$$\lambda_L \Delta t.$$

Numerical simulation

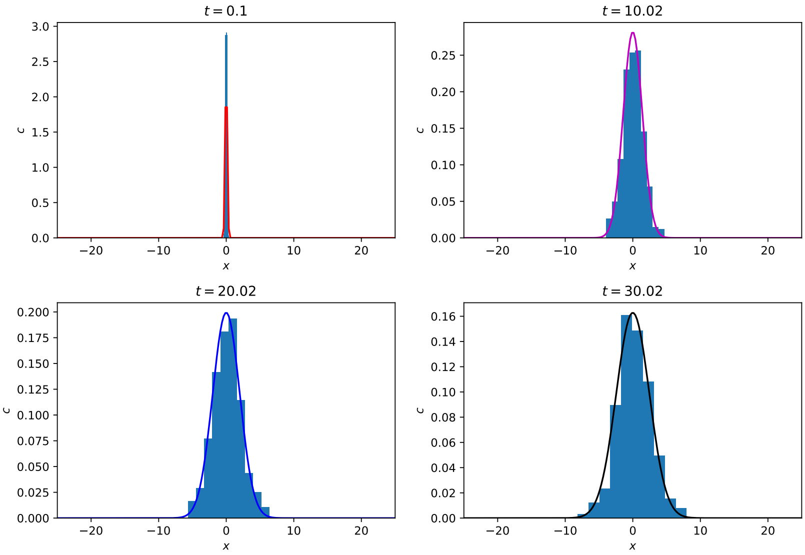

Figure 3: Numerical implementation of random walk

Derivation

Let $c(x,t)$ represent the particle density at spatial location x and time t.

A conservation equation for c is given by

$$c(x,t+\Delta t) = c(x,t) + \lambda_R \Delta t c(x-\Delta x,t) - \lambda_R \Delta t c(x,t) + \\ \lambda_L \Delta t c(x+\Delta x,t) - \lambda_L \Delta t c(x,t).$$