

Lecture slides

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Lecture 1

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

Conservation equations

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

Spatially homogeneous models (MA32009 revision)

Example problem - bacteria in a dish

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

A model for cell growth under nutrient depletion

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

Leading to the logistic growth equation

The last equation can be rewritten as

$$\frac{dN}{dt} = \rho N \left(1 - \frac{N}{B}\right) \quad N(0) = N_0, \quad (2)$$

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

i Model checklist

1. Variables (dependent, independent ?)
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

Consider a well mixed bio reactor.

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

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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

$$\frac{dS}{dt} = -rIS,$$

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

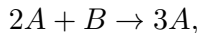
$$\frac{dR}{dt} = aI.$$

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



with reaction rate k_3 .

Write down governing ODEs.

Activator-inhibitor model

Consider the ODEs

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

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:

$$\begin{aligned} \left(\begin{array}{c} \text{rate of change of} \\ \text{number of particles} \\ \text{per unit time} \end{array} \right) &= \left(\begin{array}{c} \text{rate of entry of} \\ \text{particles into } V \\ \text{per unit time} \end{array} \right) - \left(\begin{array}{c} \text{rate of exit of} \\ \text{particles from } V \\ \text{per unit time} \end{array} \right) \\ &\quad + \left(\begin{array}{c} \text{rate of degradation} \\ \text{or creation of particles} \\ \text{in } V \text{ per unit time} \end{array} \right) \end{aligned}$$

Deriving a conservation equation in 1D

$$\begin{aligned} \frac{\partial}{\partial t} \int_x^{x+\Delta x} c(\tilde{x}, t) A d\tilde{x} &= J(x, t) A - J(x + \Delta x, t) A \\ &+ \int_x^{x+\Delta x} f(\tilde{x}, t, c(\tilde{x}, t)) A d\tilde{x}. \end{aligned} \quad (3)$$

A conservation PDE in 1D

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

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

$$\mathbf{J} = -D\nabla c, \quad (5)$$

Fluxes - Nonlinear diffusion

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

Hence

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

Fluxes - Convection/advection

$$\mathbf{J} = \mathbf{v}c, \quad (6)$$

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

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

so in 1D Cartesian coordinates

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

1D diffusion equation with delta IC

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

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

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

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

Numerical solution

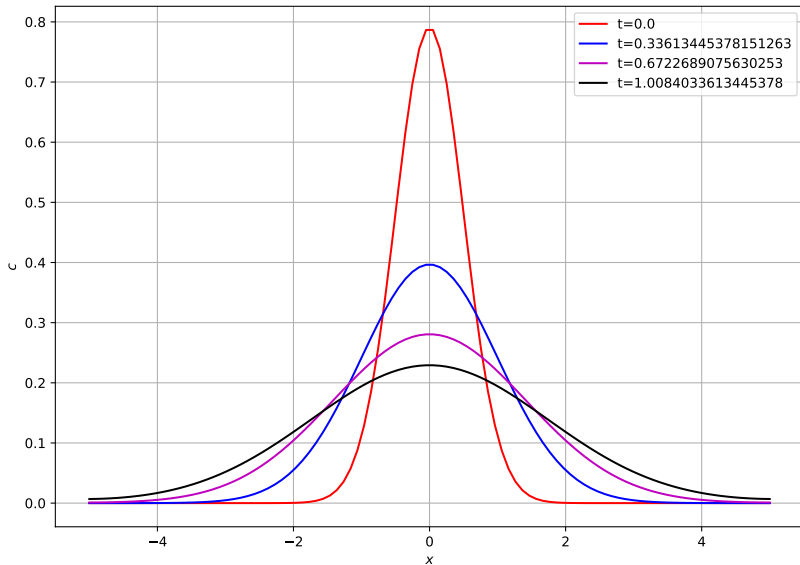


Figure 1: Numerical solution of diffusion equation.

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

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

The 1D diffusion equation for arbitrary initial condition

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

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

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

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

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

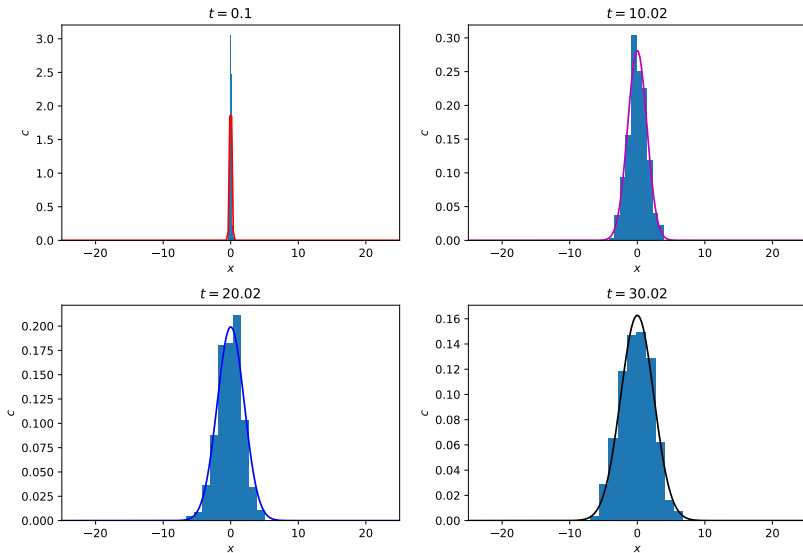


Figure 3: Numerical implementation of random walk

Derivation

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

A conservation equation for c is given by

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

Lecture 6

- ▶ Random walk as a model for the diffusion equation
- ▶ Linear reaction diffusion

Recap from last week

A conservation equation for c is given by

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

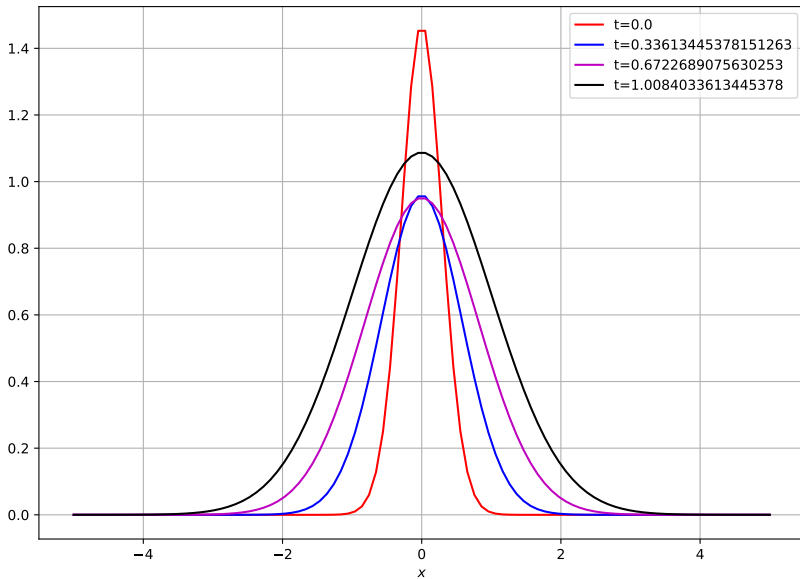
Linear reaction term

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + \rho c, \quad x \in \mathbb{R}, \quad t > 0, \quad (10)$$

where $\rho \in \mathbb{R}$ is a constant. with initial condition

$$u(x, 0) = M\delta_0(x), \quad x \in \mathbb{R}. \quad (11)$$

Numerical solution



Muskrat invasion dynamics

$$\frac{\partial u}{\partial t} = D \left(\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2} \right) + \rho u, \quad \mathbf{x} = (x_1, x_2) \in \mathbb{R}^2, \quad t > 0,$$

with initial condition

$$u(\mathbf{x}, 0) = M \delta_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2. \quad (12)$$

$$u_1(\mathbf{x}, t) = \frac{M}{4\pi Dt} \exp \left(\rho t - \frac{r_1^2}{4Dt} \right).$$