MA42002

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Introduction

Welcome to MA42002 Mathematical Biology II.

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Lecture notes

You can find lecture notes for the module on this page. If you would like a pdf this can be easily generated by clicking on the pdf link on the top left of the webpages. I will occasionally edit/update the notes as we proceed through lectures. If you spot any errors/typos/inconsistencies/omissions etc. please report an issue using the report an issue link on the right-hand side of the webpages.

Reading

Mathematical Biology II, James Dickson Murray (2003)

Python codes

I have provided Python codes for most of the figures in the html version of the notes (you can unfold code section by clicking 'Code'). Note that the Python code does not appear in the pdf.

Many of you have taken the Introduction to Programming module at Level 2 and have therefore some experience using Python. I strongly encourage you to use the provided codes as a tool to play around with numerical solutions of the various models that we will be working on. The codes should run as standalone Python codes.

Plan

Table 1: Projected delivery

Week	Chapter	Tutorial sheet
1	1	1
2	2	1
3	3	2
4	3	2
5	4	3
6	4	4
7	5	4
8	5	5
9	6	5
10	6	6
11	7	6

References

1 Conservation equations

1.1 Introduction

Many biological systems are spatio-temporal, i.e. concentrations of biochemicals, densities of cells etc. depend on spatial position as well time. To describe such cases we must *relax* a major assumption that was made in Mathematical Biology I (MA32009): spatial homogeneity. We now models biological system using partial differential equations.

A conservation equation is the most fundamental statement through which changes in the distribution of the density (or concentration, temperature) is described.

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

1.1.1 Notation

We will consider $x \in \mathbb{R}^n$, $t \in [0, \infty)$ and functions $c : \mathbb{R}^n \times [0, \infty) \to \mathbb{R}$, where $n = 1, 2, 3$. For example:

- $c(x, t)$ - the density of a population [number per volume] at position x and time t (at (x, t))
- $c(x, t)$ - the concentration of a substance (chemicals, particles) [mass per volume] at position x and time t (at (x, t))
- $c(x, t)$ - the temperature at (x, t).

1.2 Spatially homogeneous models

In this section, we neglect spatial movement and consider examples of growth/death and chemical reactions (i.e. revision from MA32009).

1.2.1 Population dynamics

1.2.1.1 Modelling the growth of bacteria in a petri dish (flask) containing nutrient medium

As an example let's consider a population of bacteria growing in a bounded domain (e.g. a petri dish).

Bacteria reproduce by undergoing successive cell divisions.

Let $N(t)$ represent bacterial density at time t (i.e. number of cells per volume).

Let K represent the *per capita* rate of reproduction. Over a period of time, Δt, $KN(t)\Delta t$ cells will be added. Hence

$$N(t+\Delta t) = \quad N(t) + \quad KN(t)\Delta t. \tag{1.1}$$

Assuming that N is differentiable, dividing Equation **??** by Δt and taking the limit as $\Delta t \to 0$

$$\frac{dN}{dt} = KN. \tag{1.2}$$

Depending on the biological context, the growth rate K may take several forms e.g.

- $K =$ constant
- $K = K(t)$ time-dependent
- $K = K(N(t))$ depends on bacterial density
- $K = K(c(t)) := \kappa c(t)$, (with $\kappa > 0$ a constant), which depends on the nutrient concentration $c(t)$ at time t.

1.2.1.2 Logistic growth via nutrient depletion

Suppose that the population growth rate depends on nutrient availability. Suppose also that nutrient levels are depleted by population growth.

Let $c(t)$ represent the nutrient concentration at time, t. Based on the above assumptions we derive

$$\begin{aligned} \frac{dN}{dt} &= K(c)N = \kappa cN, \\ \frac{dc}{dt} &= -\alpha\frac{dN}{dt} = -\alpha\kappa cN, \end{aligned} \tag{1.3}$$

where κ and $\alpha \in \Re$. Consider the initial conditions

$$N(0) = N_0 \quad \text{and} \quad c(0) = c_0.$$

Noting the conserved quantity

$$\alpha\frac{dN}{dt}+\frac{dc}{dt}=0,$$

integration yields

$$c(t)=-\alpha N(t)+c(0)+\alpha N(0)=-\alpha N(t)+\beta, \tag{1.4}$$

where $\beta=c_0+\alpha N_0$. Substituting for Equation **??** in Equation **??** we obtain the *logistic growth* equation

$$\frac{dN}{dt}=\kappa(\beta-\alpha N)N, \qquad N(0)=N_0 \quad , \tag{1.5}$$

where $K=K(N)=\kappa(\beta-\alpha N)$.

The last equation can be rewritten as

$$\frac{dN}{dt}=\rho N\,(1-\frac{N}{B}) \qquad N(0)=N_0, \tag{1.6}$$

where $\rho=\kappa\beta$ is the *intrinsic growth rate* and $B=\frac{\beta}{\alpha}$ is the *carrying capacity*. The solution of Equation **??** is given by

$$N(t)=\frac{N_0K}{N_0+(B-N_0)e^{-\rho t}}\ .$$

1.2.1.3 Death/decay

In addition to growth, we may assume that cells die at rate d and the simple growth Equation **??** can be generalised to

$$\frac{dN}{dt}=KN-dN,$$

where d is the mortality (death) rate.

1.2.1.4 Competition

Consider a situation in which the *per capita* death rate increases at higher density. For example, suppose that

$$d=d_1N,$$

i.e. the mortality (death) rate is proportional to the population density. This assumption might arise in a situation where individuals compete for food, habitat (i.e. space) or any limited resources. Hence we could obtain the nonlinear ODE

$$\frac{dN}{dt}=KN-d_1N^2,$$

1.2.2 SIR Model

Consider a model of infectious disease in which a population is split into three compartments:

- susceptible
- infected
- recovered

Suppse that when susceptible and infected individuals interact, the susceptibles become infected. Suppose also that infected people only remain infectious for a limited time.

Let $S(t)$, $I(t)$ and $R(t)$ represent the population densities of susceptible, infected and recovered populations, respectively.

Consider the governing ODE

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

where r is the infection rate and a is the recovery rate.

1.2.3 Activator inhibitor kinetics

Consider a pair of interacting biochemical species, A and B. Suppose that both A and B are produced at a constant rate and that A undergoes linear degradation. Suppose also that A and B interact such that

$$2A + B \to A.$$

Applying the law of mass action

$$\begin{aligned}\frac{dA}{dt} &= k_1 - k_2 A + k_3 A^2 B,\\ \frac{dB}{dt} &= k_4 - k_3 A^2 B,\end{aligned}$$

where k_1 and k_4 are production rates, k_2 is a degradation rate and k_3 is the reaction rate for the A and B interaction.

1.3 Spatial movement

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:

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

1.3.1 One-dimensional conservation equations

Assume

- motion takes place in a one-dimensional domain (e.g. a long very thin tube)
- the tube has a constant cross-section area

Let x be the distance along the tube relative to an origin. We shall consider the interval $(x + \Delta x, t)$, for some $\Delta x > 0$, and a domain $V = (x, x + \Delta x) \times S$, where S is the cross-section of the tube with the constant area $A = |S|$.

- $c(x, t)$ - concentration of particles (number of particles per unit volume) at time, t, and position, x
- $J(x, t)$ - flux of particles per unit time and unit area (number of particles crossing a unit area in the positive x-direction per unit time)
- $f(x, t, c(x, t))$ - source/sink (number of particles created or destroyed per unit volume and unit time)

We consider S to be very small and $c(x, t)$ is assumed to be constant in S (independent of y and z). We also assume that c is continuously differentiable with respect to t.

The volume of V is $A\Delta x$ and number of particles in the volume is given by

$$\int_x^{x+\Delta x} c(\tilde{x}, t)\, d\tilde{x} A.$$

Then a conservation equation for the number of particles in the volume V is given by

$$\frac{\partial}{\partial t}\int_x^{x+\Delta x} c(\tilde{x}, t) A d\tilde{x} = J(x, t)\, A - J(x + \Delta x, t)\, A + \int_x^{x+\Delta x} f(\tilde{x}, t, c(\tilde{x}, t))\, A\, d\tilde{x}. \qquad (1.7)$$

i.e. the flux that changes the total population in V is that entering through the cross-section at x and leaving through the cross-section at $x + \Delta x$ (it is assumed that there no flux through

the external surface of the tube). Assuming c and f to be sufficiently smooth (continuous in x) and applying The Mean Value Theorem in Equation **??**, we obtain

$$\frac{\partial}{\partial t}c(\xi,t)A\Delta x = J(x,t)\,A - J(x+\Delta x,t)\,A + f(\eta,t,c(\eta,t))\,A\Delta x, \qquad \xi,\eta\in(x,x+\Delta x). \tag{1.8}$$

Dividing Equation **??** by $A\,\Delta x$ yields

$$\frac{\partial}{\partial t}c(\xi,t) = -\frac{J(x+\Delta x,t)-J(x,t)}{\Delta x} + f(\eta,t,c(\eta,t)), \qquad \xi,\eta\in(x,x+\Delta x). \tag{1.9}$$

Assuming that J is differentiable with respect to x and taking the limit as $\Delta x\to 0$ (and using the definition of partial derivatives) we obtain a one-dimensional conservation (balance) equation:

$$\frac{\partial}{\partial t}c(x,t) = -\frac{\partial}{\partial x}J(x,t) + f(x,t,c(x,t)). \tag{1.10}$$

1.3.2 Conservation equations in $\mathbb{R}^n$

Let $V\subset\mathbb{R}^n$ be an arbitrary bounded domain (i.e. satisfying the conditions of the divergence theorem) and let S be the surface enclosing V, i.e $S=\partial V$.

- $c(x,t)$ – concentration of particles at $x\in V$ and $t>0$ (number of particles per unit volume)
- $J(x,t)$ – flux vector of particles across V (number of particles per unit area and per unit time entering or leaving through S (the boundary of V).
- $f(x,t,c(x,t))$ - source/sink term (number of particles created or destroyed per unit volume and per unit time)

Then the conservation equation reads

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

where $\mathbf{n}$ is the outward normal vector to S. The normal component of the flux J on S leads to a change of number of particles (of mass) in V. Applying the divergence theorem, i.e.

$$\int_S J\cdot\mathbf{n}\,d\sigma = \int_V \mathrm{div}J\,dx,$$

and using the fact that V is independent of time t we obtain

$$\int_V \Big(\frac{\partial}{\partial t}c(x,t) + \nabla\cdot J(x,t) - f(x,t,c)\Big)dx.$$

Since V can be chosen arbitrary we get the conservation equation in $\mathbb{R}^n$ (or a subdomain $\Omega\subset\mathbb{R}^n$)

$$\frac{\partial}{\partial t}c(x,t) = -\nabla \cdot J(x,t) + f(x,t,c), \quad x \in \mathbb{R}^n \text{ (or } x \in \Omega), \quad t > 0. \tag{1.11}$$

1.3.3 Types of flux terms

- Fickian Diffusion

  Diffusion is an important and ''metabolically cheap" transport mechanism in biological systems. It can be also viewed as the random motion of individual molecules.

  $$\mathbf{J} = -D\nabla c, \tag{1.12}$$

  where D is the diffusion coefficient. D depends on the size of the particles, the type of solvent, the temperature, ….

  Then applying Equation **??** in Equation **??** we obtain reaction-diffusion equation

  $$\frac{\partial}{\partial t}c = -\nabla \cdot (-D\nabla c(x,t)) + f(x,t,c) = \nabla \cdot (D\nabla c) + f(x,t,c), \quad x \in \mathbb{R}^n, \ t > 0. \tag{1.13}$$

  If D is a constant we can write

  $$\frac{\partial}{\partial t}c(x,t) = D\Delta c(x,t) + f(x,t,c), \quad x \in \mathbb{R}^n \text{ (or } x \in \Omega), \quad t > 0,$$

  where

  $$\Delta c = \sum_{j=1}^{n} \frac{\partial^2 c}{\partial x_j^2}.$$

- Nonlinear diffusion

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

  and

  $$\frac{\partial}{\partial t}c = D_0 \nabla \cdot (c^m \nabla c) + f(x,t,c), \quad x \in \mathbb{R}^n, \quad t > 0. \tag{1.14}$$

- Convection or advection

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

  where $\mathbf{v}$ is a velocity vector. Hence

  $$\frac{\partial}{\partial t}c(x,t) = -\nabla \cdot (\mathbf{v}(x,t)c(x,t)) + f(x,t,c), \quad x \in \mathbb{R}^n, \quad t > 0. \tag{1.15}$$

  If $\mathbf{v}$ is constant or $\nabla \cdot \mathbf{v} = 0$, then

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

- Taxis - directed movement in response to an external chemical or physical signal.
  - chemotaxis - movement directed by a chemical gradient
  - haptotaxis - movement directed by a gradient in density, adhesion

  In the presence of some chemoattractant $a(x,t)$ we have

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

  where $\chi(a)$ is a 'model-specific' function of a defining the sensitivity to the signal, and the conservation equation reads

$$\frac{\partial}{\partial t} c(x,t) = -\nabla \cdot (\chi(a) c(x,t) \nabla a) + f(x,t,c), \quad x \in \mathbb{R}^n \quad t > 0. \tag{1.16}$$

1.3.4 Boundary conditions (B.C.)

- Infinite domain (e.g. $(-\infty, \infty)$, $\mathbb{R}^2$, $\mathbb{R}^3$):

the density is not influenced by the boundary

$$c(x,t) \to 0 \qquad \text{as} \qquad \|x\| \to \infty \quad \text{decay at infinity}$$

- Periodic B.C.

L-periodic function: $c(x,t) = c(x, t+L)$ for any x in the domain

Consider a domain $(0, L)$.

$$c(t,0) = c(t,L) \qquad \text{periodic boundary conditions}$$

- Dirichlet B.C.

density (concentration) is fixed at the boundary

In the 1-dim domain $(0, L)$

$$c(t,0) = c_1, \quad c(t,L) = c_2$$

can consider two reservoirs placed at the ends of the domain, that are held at constant densities (concentrations) c_1 and c_2, respectively.

For a domain $\Omega \subset \mathbb{R}^n$ we have

$$c(x,t) = c_D(x,t) \qquad x \in \partial\Omega, \ t \geq 0 \ .$$

- No-flux (homogeneous Neumann) B.C.

particles cannot escape from the domain

For a domain $\Omega \subset \mathbb{R}^n$

$$D\nabla c \cdot \mathbf{n} = 0 \quad \text{on} \quad \partial\Omega, \quad t > 0$$

In one-dimensional domain $(0, L)$

$$\frac{\partial c(x,t)}{\partial x} = 0 \quad \text{at} \quad x = 0 \text{ and } \quad x = L, \quad t > 0\ ,$$

- Non-homogeneous Neumann B.C.

For a domain $\Omega \subset \mathbb{R}^n$

$$D\nabla c \cdot \mathbf{n} = g(x,t) \quad \text{on} \quad \partial\Omega, \quad t > 0$$

with a given function g (g can also be a constant).

In one-dimensional domain $(0, L)$

$$D\frac{\partial c(x,t)}{\partial x} = g(x,t) \quad \text{at} \quad x = 0 \text{ and } \quad x = L, \quad t > 0\ ,$$

- Homogeneous Robin B.C.

$$D\nabla c(x,t) \cdot \mathbf{n} + kc(x,t) = 0 \quad \text{on} \quad \partial\Omega, \quad t > 0$$

with some constant $k \in \mathbb{R}$.

In one-dimensional domain $(0, L)$

$$D\frac{\partial c(x,t)}{\partial x} + kc(x,t) = 0 \quad \text{at} \quad x = 0 \text{ and } \quad x = L, \quad t > 0\ ,$$

- Non-homogeneous Robin B.C.

$$D\nabla c(x,t) \cdot \mathbf{n} + kc(x,t) = g(x,t) \quad \text{on} \quad \partial\Omega, \quad t > 0$$

with some constant $k \in \mathbb{R}$ and given function g (g can also be a constant).

In one-dimensional domain $(0, L)$

$$D\frac{\partial c(x,t)}{\partial x} + kc(x,t) = g(x,t) \quad \text{at} \quad x = 0 \text{ and } \quad x = L, \quad t > 0\ ,$$

Remark We can also have different types of boundary conditions at different parts of the boundary of the considered domain.

1.3.5 Initial conditions

For a conservation equation defined in a domain $\Omega \subset \mathbb{R}^n$, $n = 1, 2, 3$, additionally to boundary conditions we need to define an initial concentration, i.e. initial condition

$$c(0, x) = c_0(x), \qquad x \in \Omega \, .$$

1.3.6 Formulating a model

The models that we will consider will comprise one or more partial differential equations together with boundary and initial conditions. The right-hand side of the PDEs will be derived based upon assumptions about a particular biological system under study. We will consider exploratory numerical solutions and then study qualitative behaviours of the solutions using analyses familiar from MA32009 (e.g. steady state analysis, linear stability analysis).

We can have any combination of fluxes, depending on the biological system. For example, chemotaxis and diffusion

$$\frac{\partial}{\partial t} c = D\Delta c - \nabla \cdot (\chi(a) c \nabla a) + f(x, t, c), \quad x \in \mathbb{R}^n \quad t > 0, \tag{1.17}$$

which can be augmented by an equation for the (diffusible) chemoattractant a

$$\frac{\partial}{\partial t} a = D\nabla^2 a + g(x, t, a, c), \quad x \in \mathbb{R}^n \quad t > 0. \tag{1.18}$$

Equation **??** and Equation **??** form a system of equations, a so-called chemotaxis system.

i Checklist

Depending on the problem under study, you will have to define and justify your use of the following:

1. Independent variables
2. Dependent variables
3. Domain of definition
4. Reaction kinetics
5. Fluxes
6. Initial conditions
7. Boundary conditions

1.3.7 Nondimensionalization

The variables and parameters in a biological or physical model have units:

- $\#\text{velocity} = \dfrac{\#\text{length}}{\#\text{time}}$
- $\#\text{concentration} = \dfrac{\text{num.moles}}{\#\text{volume}}$
- $\#\text{density} = \dfrac{\text{number of particles}}{\#\text{volume}}$
- $\#\text{diffusion coefficient} = \dfrac{\#\text{length}^2}{\#\text{time}}$
- $\#\text{source/sink (reaction term)} = \dfrac{\#\text{concentration (or density)}}{\#\text{time}}$
- $\#\text{flux} = \dfrac{\text{mass (number) of particles}}{\#\text{area} \times \#\text{time}}$

It is standard to non-dimensionalise a system of differential equations by scaling or non-dimensionalising both the dependent and independent variables in the model.

Part I

Single species

2 Linear reaction diffusion equations

We will now consider equations (and systems of such equations) of the general form:

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

Such an equation is known as a *reaction-diffusion equation*, being composed of a reaction term, $f(c)$, and a diffusion term, $D\nabla^2 c$. Reaction-diffusion equations have many applications in biological systems e.g. travelling waves of invasion, pattern formation, spread of infectious diseases. For most of the remainder of the course we will consider such systems in one-space dimension i.e. $x \in \mathbb{R}$.

Consider the one-dimensional reaction-diffusion equation with constant diffusion coefficient $D > 0$:

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

2.1 One-dimensional diffusion equations

In order to provide some insight into the structure of solutions of reaction-diffusion equations, we make an initial simplifying assumption i.e. we assume $f(c) = 0$, and obtain the linear diffusion equation (or heat equation):

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}, \quad x \in \mathbb{R}, \;\; t > 0. \tag{2.1}$$

This equation is used to model the evolution of the concentration of a chemical in a long thin tube, or the temperature of a long thin rod.

We assume that the solution is initialised to be non-zero at one point $x = 0$, i.e.

$$c(x_0, 0) = \delta_0(x) \qquad x \in \mathbb{R}, \tag{2.2}$$

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

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

2.1.1 Fundamental solution

It can be shown that the sequence of functions $\{\phi_\varepsilon(x)\}$ given by

$$\frac{1}{\varepsilon\sqrt{\pi}} e^{-\frac{x^2}{\varepsilon^2}}$$

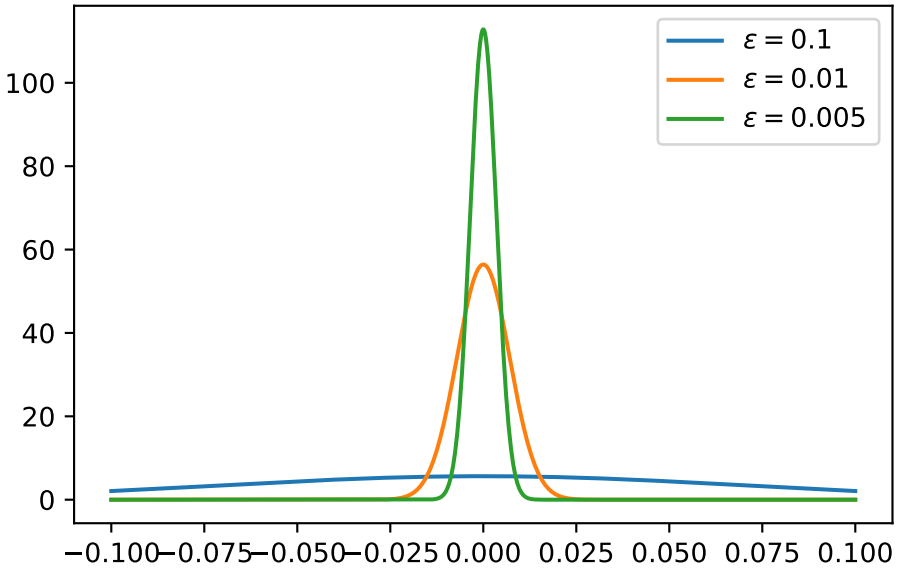

Figure 2.1: Approximation of Dirac delta function.

converges to $\delta_0(x)$ as $\varepsilon \to 0$ (in the sense of distributions or generalized functions).

Then for the diffusion Equation **??** with initial condition Equation **??**, it can be shown that the explicit (analytic) solution is given by

$$c(x,t) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right). \tag{2.3}$$

This is known as the *fundamental* solution of the diffusion equation in $\mathbb{R}$.

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

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

This result can be generalized to $\mathbb{R}^n \times (0,\infty)$ where the fundamental solution has the form

$$c(x,t) = \frac{1}{(4\pi Dt)^{n/2}} \exp\left(-\frac{(x_1^2 + x_2^2 + \ldots + x_n^2)}{4Dt}\right).$$

2.1.2 Numerical solution

In Figure **??** we compute a numerical solution of the diffusion equation and compare it with the exact solution given by Equation **??**.

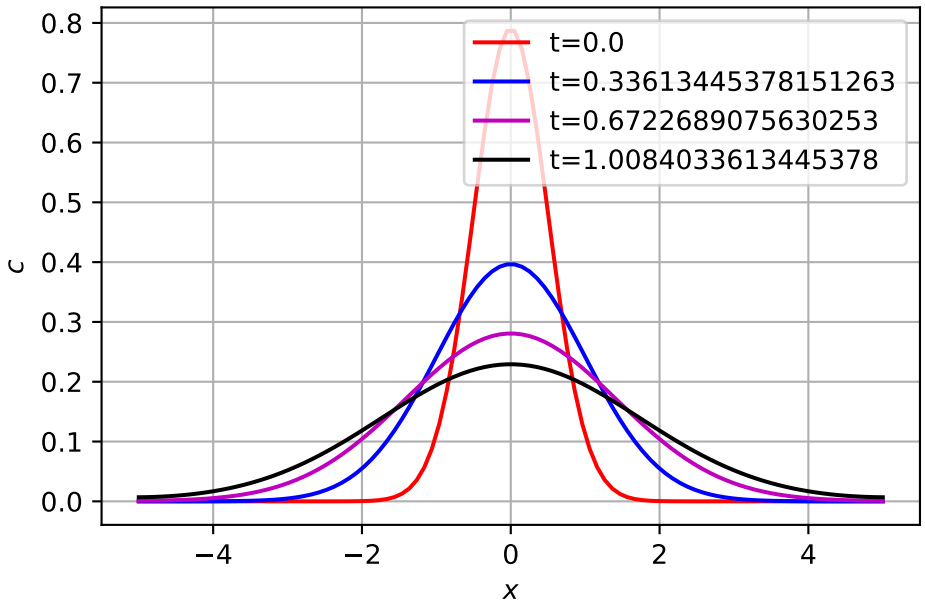

Figure 2.2: Numerical solution of diffusion equation.

2.1.3 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).

2.1.4 Diffusive transit time

We now demonstrate the connection between time and space in diffusion equations Consider particles of concentration $c(x,t)$ diffusing with constant diffusion D in a one-dimensional domain $(0,L)$, with a constant concentration at one boundary and removed by a sink at the other boundary. At steady-state, the equation governing the concentration is given by:

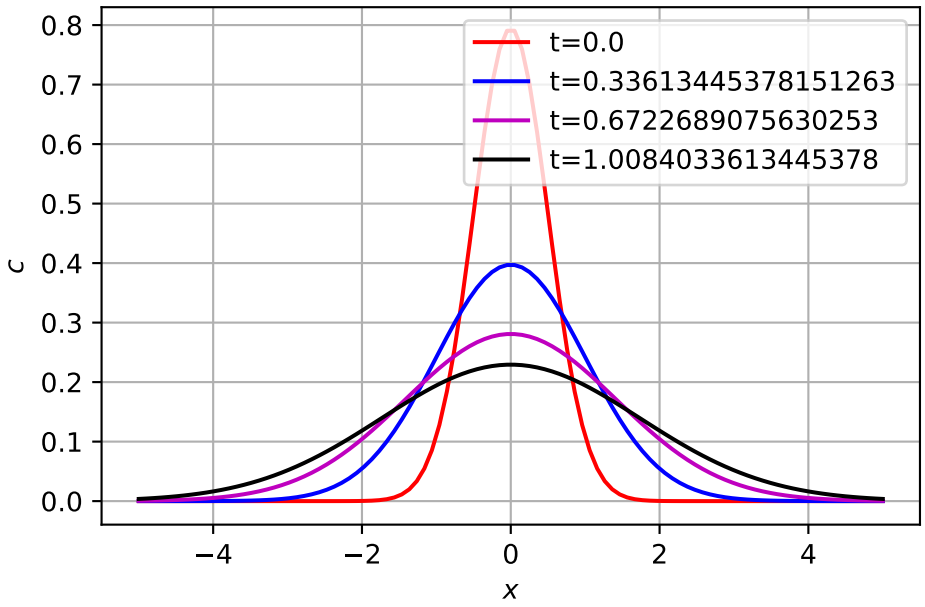

Figure 2.3: Exact solution of diffusion equation.

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

The solution (**Exercise**) is:

$$c(x) = C_0\left(1 - \frac{x}{L}\right).$$

Then the number of particles entering at $x = 0$ due to diffusive flux (Fickian diffusion) is:

$$J = -D\frac{dc}{dx} = D\frac{C_0}{L},$$

In the middle of the domain the particle concentration is

$$c(\frac{L}{2}) = \frac{C_0}{2}.$$

A typical particle speed is approximated by

$$\frac{J}{c} = \frac{D\frac{C_0}{L}}{\frac{C_0}{2}} = \frac{2D}{L}$$

Travelling at this speed, the average time it takes a particle to travel a distance, L, is

$$\tau = \frac{\text{distance}}{\text{speed}} = \frac{L^2}{2D.}$$

Hence the average distance through which diffusion transports a particle in a time τ is $L = \sqrt{2D\tau}$.

2.1.5 Diffusion as the limit of a random walk

Consider the *random walk* of particles in a one-dimensional domain. Suppose that the particles move randomly a distance, Δx, every time step, Δt. Assume that the particles move left with probability λ_L and right with probability λ_R.

In Figure **??** a simulation of 400 random walking particles is presented. Each particle is initialised at the origin and can move one step left or right with equal probability at every time step of the simulation. As time evolves the particle density (histogram) disperses. The normalised particle density appears to be well described by the solution of the diffusion equation (solid lines, Equation **??**).

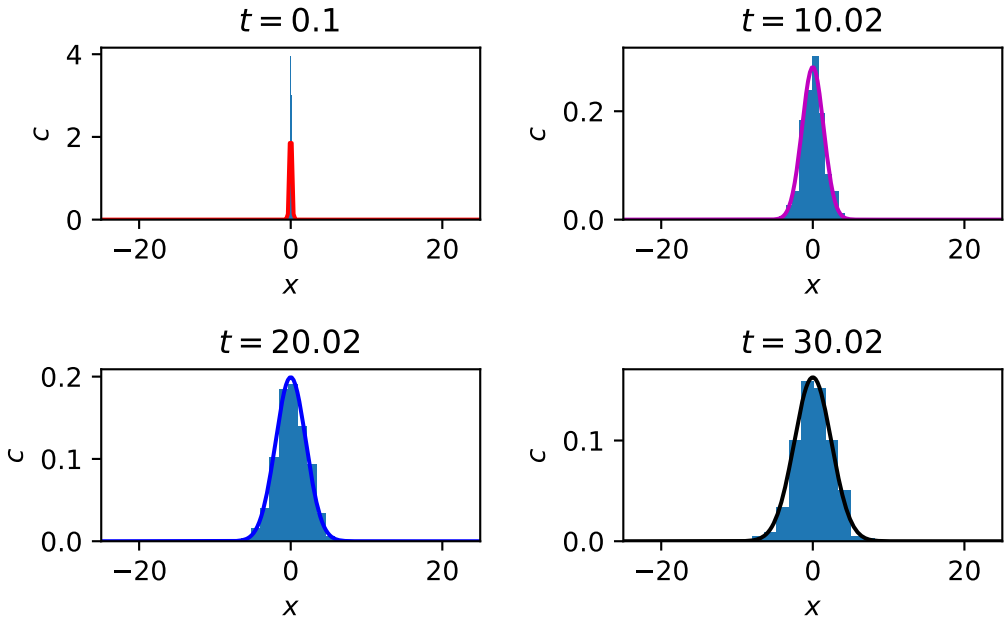

Figure 2.4: Numerical implementation of random walk

Consider the concentration of particles $c(x,t)$ at spatial location x and time t, (or more precisely, the probability density function of the position of a particle performing a random walk)

we have:

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

If we assume that $\lambda_R + \lambda_L = 1$ then

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

Applying a Taylor series expansion about (x, t) implies

$$c(x,t)+\frac{\partial c}{\partial t}\Delta t+\frac{1}{2}\frac{\partial^2 c}{\partial^2 t}(\Delta t)^2+h.o.t. = \lambda_R\Big(c(x,t)-\frac{\partial c}{\partial x}\Delta x+\frac{1}{2}\frac{\partial^2 c}{\partial^2 x}(\Delta x)^2+h.o.t.\Big)+\lambda_L\Big(c(x,t)+\frac{\partial c}{\partial x}\Delta x+\frac{1}{2}\frac{\partial^2 c}{\partial^2 x}(\Delta x)^2-$$

Using $\lambda_R + \lambda_L = 1$ and assuming $\lambda_L = \lambda_R = \frac{1}{2}$ we obtain

$$\frac{\partial c}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 c}{\partial^2 t}(\Delta t)^2 + h.o.t. = \frac{1}{2}\frac{\partial^2 c}{\partial^2 x}(\Delta x)^2 + h.o.t.$$

Dividing by Δt gives

$$\frac{\partial c}{\partial t} + \frac{1}{2}\frac{\partial^2 c}{\partial^2 t}\Delta t + h.o.t. = \frac{\partial^2 c}{\partial^2 x}\frac{(\Delta x)^2}{2\Delta t} + h.o.t.$$

Considering the limit $\Delta t \to 0$ and $\Delta x \to 0$ in such way that

$$\frac{(\Delta x)^2}{2\Delta t} \to D,$$

yields the (one-dimensional) diffusion equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}.$$

This approach can be extended to consider other types of movement e.g. convection. For example, if we assume that

$$\lambda_R + \lambda_L = 1,$$

and

$$\lambda_L - \lambda_R = \varepsilon,$$

the motion of the particles is biased and we may derive an appropriate *reaction-diffusion-convection* equation (see tutorial).

Finally we note that there is a connection between diffusion and the normal distribution function.

Recall The normal distribution function in one-dimension with zero mean and variance σ^2 is given by

$$N(0, \sigma^2) \sim \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right).$$

Examining the formula for the fundamental solution of the diffusion Equation **??** in one-dimension, we see by inspection that the probability density function of the position of a particle performing a random walk in one-dimension starting at the origin is normally distributed with mean zero and variance

$$\sigma^2 = 2Dt.$$

2.2 Linear reaction-diffusion equations

Consider now the linear reaction term: $f(c) = \rho c$, so that our reaction-diffusion equation is:

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} + \rho\, c, \quad x \in \mathbb{R},\ t > 0, \tag{2.4}$$

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

Once again we consider the initial condition to be concentrated at the origin:

$$c(0, x) = \delta_0(x). \tag{2.5}$$

2.2.1 Exact solution

By considering a *separation of variables* approach, i.e. making the *ansatz*

$$c(x, t) = w(t)\tilde{c}(t, x),$$

it can be shown (**Exercise**) that the explicit solution for the linear reaction-diffusion Equation **??** with initial condition Equation **??** is given by

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

In Figure **??** we compare numerical and exact solutions.

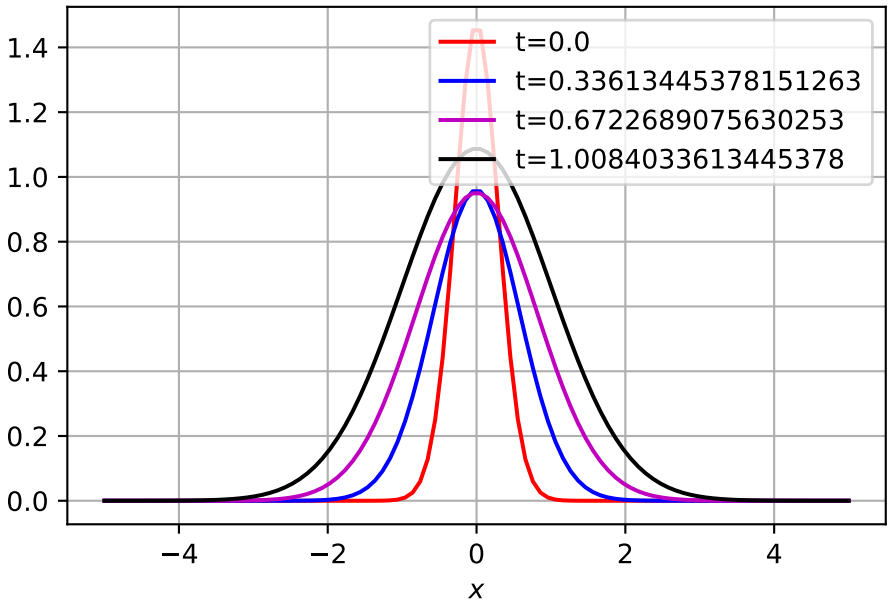

Figure 2.5: Numerical solution of linear reaction diffusion equation

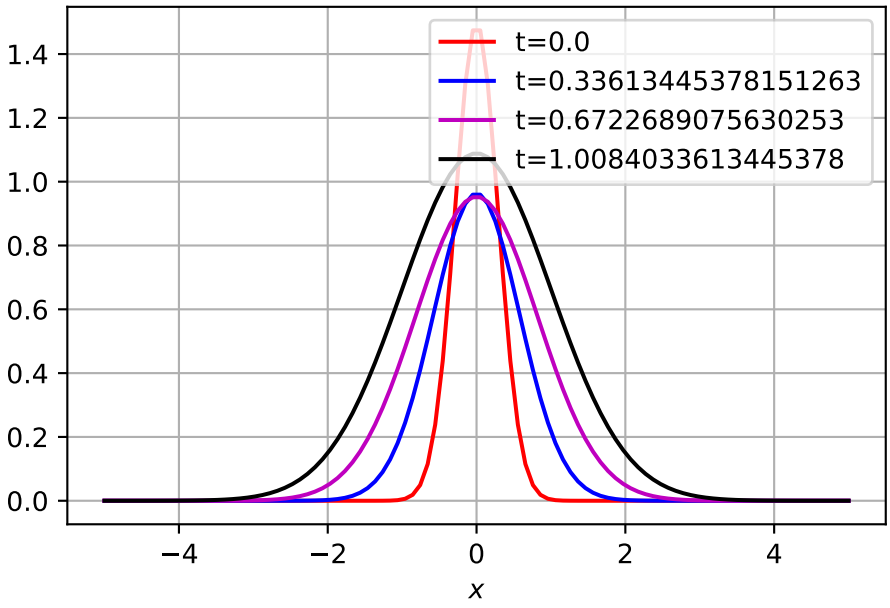

Figure 2.6: Exact solution of linear reaction diffusion equation

2.2.2 Speed of a wave of invasion

Muskrats which were introduced in 1905 in Bohemia initially spread rapidly throughout Europe through a combination of random movement and proliferation (initially there were no predators and proliferation was rapid). A model for the initial spread can therefore be given by a two-dimensional diffusion equation combined with exponential growth and assuming that M individuals were released at the origin (i.e. in Bohemia). Considering the density of muskrats $u(\mathbf{x}, t)$, the equation is

$$\frac{\partial u}{\partial t} = D\left(\frac{\partial^2 u}{\partial x_1^2} + \frac{\partial^2 u}{\partial x_2^2}\right) + \rho\, u, \quad \mathbf{x} = (x_1, x_2) \in \mathbb{R}^2,\ t > 0, \tag{2.6}$$

$$u(\mathbf{x}, 0) = M\delta_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2. \tag{2.7}$$

The solution of Equation **??** with initial conditions Equation **??** is equal to:

$$u(\mathbf{x}, t) = \frac{M}{4\pi D t} \exp\left(\rho t - \frac{|\mathbf{x}|^2}{4Dt}\right) = \frac{M}{4\pi D t} \exp\left(\rho t - \frac{(x_1^2 + x_2^2)}{4Dt}\right).$$

Transforming to polar coordinates $x_1 = r\cos\varphi$, $x_2 = r\sin\varphi$ we obtain

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

From the properties of the fundamental solution, the wave of invasion extends all the way to infinity if $t > 0$. Thus, for practical purposes, somehow we have to define the front of the wave.

Consider that there is some detection threshold for the muskrats i.e. some predetermined small value of the density u_1, say, such that any changes in density for $u < u_1$ cannot be detected.

Because of the symmetry of the problem, then the leading edge of the invading wave front of muskrats is the circle of radius $r = r_1(t)$ where $u = u_1$, i.e. from the explicit solution of Equation **??**,

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

Rearranging and solving for r_1, using the fact that

$$\lim_{t\to\infty} \frac{\ln t}{t} = 0,$$

we obtain for large t that

$$r_1(t) \approx 2\sqrt{\rho D t}.$$

Hence, the speed of invasion of the leading edge of the muskrats is given by:

$$v = \frac{r_1(t)}{t} = 2\sqrt{\rho D}.$$

3 Non linear reaction diffusion equations

sdfg

We now consider the one-dimensional diffusion equation with a non-linear reaction term of "logistic growth", to give the nonlinear reaction-diffusion equation:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + \rho u\left(1 - \frac{u}{K}\right), \qquad x \in \mathbb{R},\ t > 0, \tag{3.1}$$

with initial Condition

$$u(x, 0) = u_0(x).$$

This is known as **the Fisher equation**, and was introduced by Fisher in 1937 ("The Wave of Advance of Advantageous Genes" (1937)).

We can non-dimensionalize Equation **??** by considering the scaling

$$t^* = \rho t, \quad x^* = \sqrt{\frac{\rho}{D}}x, \quad u^* = \frac{u}{K}.$$

Dropping the asteriks we obtain the non-dimensionalized Fisher equation (**Exercise**):

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1 - u), \qquad x \in \mathbb{R},\ t > 0$$

with initial condition

$$u(x, 0) = u_0(x). \tag{3.2}$$

3.1 Numerical solutions

In Figure **??** we have computed a numerical solution to Equation **??** together with no-flux boundary conditions. See Python code for further details. The key point to note is that the numerical solutions appear to be a *travelling wave*, at successive times the solution is translated along the x axis. At long times the solution tends to $u \sim 1$ (behind the wavefront). Ahead of the front, the solution is $u \sim 0$.