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 clikcing on the pdf link on the top left of the webpages. I will occasionally edit/update the notes we proceed through lectures. If you spot any errors, typos or omissions please let me know.

Reading

Mathematical Biology II, James Dickson Murray (2003)

Python codes

I have provided Python codes for most of the figures in the notes (you can unfold code section by clicking 'Code'). 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.

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.

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

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 i.e. K depends on the available resources.

1.2.1.2 Logistic growth via depleting nutrient source

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

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

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

where κ and $\alpha \in \mathfrak{R}$. Consider the initial conditions

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

Noting the conserved quantity

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

integration yields

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

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

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

Here we have $K = K(N) = \kappa(\beta - \alpha N)$.

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

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

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

The fact that individuals compete for food, habitat (i.e. space) or any limited resources, means that an increase in the net mortality of the population may be observed under crowded conditions. Hence we could obtain

$$\frac{dN}{dt} = KN - d_1 N^2,$$

where $d = d_1 N$ is the mortality (death) rate and is proportional to the population density.

1.2.2 SIR Model

Consider a model of infectious diease in which a population is slit into three compartments:

- susceptible
- infected
- recoveered

Suppse that interaction between suspectible and infected results in infection of susceptible. 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 recoveered 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 underfgoes linear degradation. Suppose also that A and B interact

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

Applying the law of mass action we obtain the ODEs

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

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 is given by

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

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

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

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.

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

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 willbe dervied 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.

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-dimensionalize a system of differential equations by scaling or non-dimensionalizing 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 initial condition for our species c is located in 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

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

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

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

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 **??**.

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

T=10
L=10

N_x=100
N_t=120

t=np.linspace(0,T,N_t)
x=np.linspace(0,L,N_x)-L/2
```

```
D=1.5
epsilon=0.1

u_0=1/(epsilon*np.sqrt(np.pi))*np.exp(-x**2/epsilon**2)

dx=L/(N_x-1)
dt=T/(N_t-1)


def diffusionPDErhs(u,t):
    N_x=len(u)
    f=np.zeros_like(u)
    for i in range(1,N_x-1):
      f[i]=D/dx**2*(u[i-1]-2*u[i]+u[i+1])


    i=0
    f[i]=D/dx**2*(-u[i]+u[i+1])
    i=N_x-1

    f[i]=D/dx**2*(u[i-1]-u[i])
    return f

sol=odeint(diffusionPDErhs,u_0,t)


[x_mesh,t_mesh]=np.meshgrid(x,t)

c_exact=1/np.sqrt(4*np.pi*D*t_mesh)*np.exp(-x_mesh**2/(4*D*t_mesh))

fig,ax=plt.subplots()
ax.plot(x, sol[1,:], 'r')
ax.plot(x, sol[4,:], 'b')
ax.plot(x, sol[8,:], 'm')
ax.plot(x, sol[12,:], 'k')
plt.legend(['t'+ str(t[0]),'t='+ str(t[4]),'t='+ str(t[8]),'t='+ str(t[12])])
plt.xlabel('$x$')
plt.grid()
plt.show()

fig,ax=plt.subplots()
```

```
ax.plot(x, c_exact[1,:], 'r')
ax.plot(x, c_exact[4,:], 'b')
ax.plot(x, c_exact[8,:], 'm')
ax.plot(x, c_exact[12,:], 'k')
plt.legend(['t'+ str(t[0]),'t='+ str(t[4]),'t='+ str(t[8]),'t='+ str(t[12])])
plt.xlabel('$x$')
plt.grid()
plt.show()
```

```
/var/folders/m_/vc0kz_0x6ls5n4qnksq052jw0000gp/T/ipykernel_21338/4177307358.py:42: RuntimeWa

divide by zero encountered in divide

/var/folders/m_/vc0kz_0x6ls5n4qnksq052jw0000gp/T/ipykernel_21338/4177307358.py:42: RuntimeWa

invalid value encountered in multiply
```

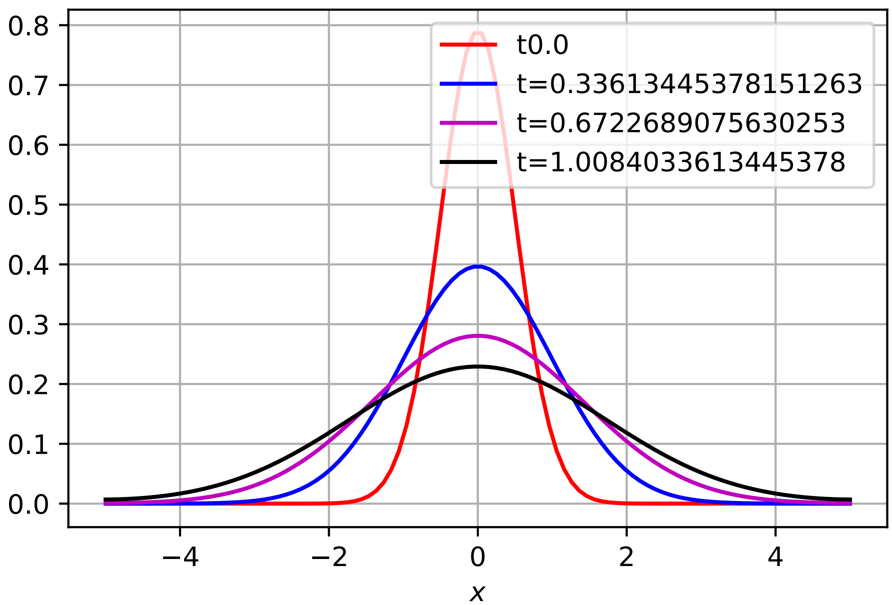

Figure 2.1: Numerical solution of diffusion equation.

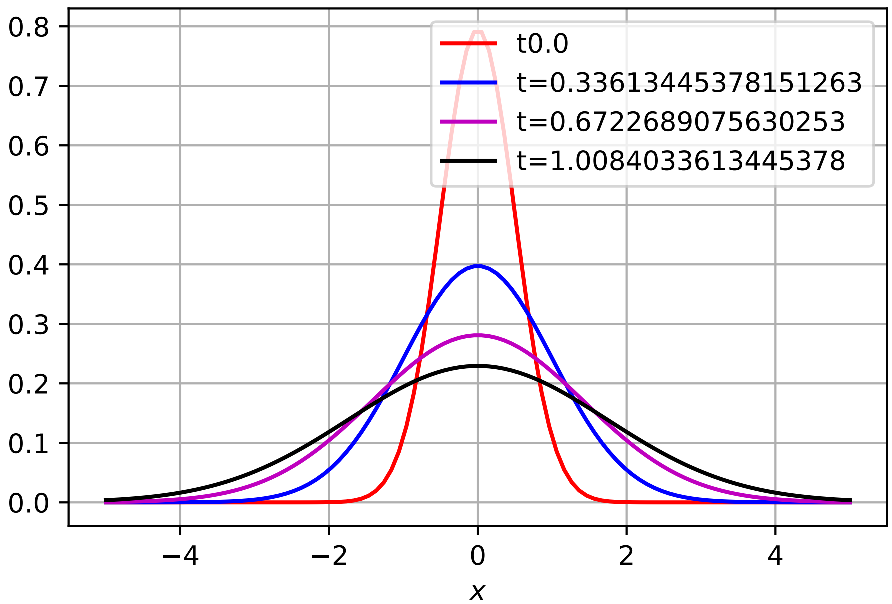

Figure 2.2: Exact solution of diffusion equation.

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 a domain $V \subset \mathbb{R}^n$, $n = 1, 2, 3.$, and particles that are entering V and are being removed from V. Define

N - total number of particles in V

F - total number of particles entering V per unit time

λ - average removal rate of particles from V

$\tau = \frac{1}{\lambda}$ - transit time or average time of residency in V

Regardless of spatial variations, we can make the following general statement regarding the total number of particles in V, where we assume a constant entry rate F and a constant removal rate λ at some sink in V:

$$\frac{dN}{dt} = \text{entry rate} - \text{removal rate} = F - \lambda N.$$

At steady state ($dN/dt = 0$) we obtain

$$Missing content here. Check notes!$$

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:

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

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:

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

and the total number of particles is given by:

$$N = \int_0^L c(x)\,dx = \frac{1}{2}LC_0.$$

If we assume a cross-section of unit area at $x = 0$, then

$$F = \text{flux} \times \text{area} = J \times 1 = D\frac{C_0}{L}$$

and

$$\tau = \frac{N}{F} = \frac{C_0 L}{2}\frac{L}{DC_0} = \frac{1}{2}\frac{L^2}{D}.$$

Thus the average time it takes a particle to diffuse a distance, L, is

$$\tau = \frac{L^2}{2D}$$

or viewed another way, 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 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 **??**).

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt
import random

N_particles=400

L=50
N_x=200

T=500
N_t=25000
D=0.1

dt=T/N_t

move_probability=D*dt/dx**2

x=np.linspace(0,L,N_x)-L/2
t=np.linspace(dt,T,N_t)

particle_positions=np.zeros((N_t,N_particles),dtype=float)

# loop over time
for i in range(1,N_t):
  # loop over particles
  for j in range(N_particles):

    r=random.random()
    # move particle j right
```

```
    new_particle_position=particle_positions[i-1,j]
    if r<move_probability:
      new_particle_position+=dx
    # move particle j left
    elif r<2*move_probability:
      new_particle_position-=dx
    particle_positions[i,j]=new_particle_position


[x_mesh,t_mesh]=np.meshgrid(x,t)
c_exact=1/np.sqrt(4*np.pi*D*t_mesh)*np.exp(-x_mesh**2/(4*D*t_mesh))


fig,ax=plt.subplots(2,2)
ax[0,0].hist(particle_positions[5,:],density=True)
ax[0,0].plot(x, c_exact[5,:], 'r')
ax[0,0].set_title('$t=$'+str(t[5]))

ax[0,1].hist(particle_positions[500,:],density=True)
ax[0,1].plot(x, c_exact[500,:], 'm')
ax[0,1].set_title('$t=$'+str(t[500]))

ax[1,0].hist(particle_positions[1000,:],density=True)
ax[1,0].plot(x, c_exact[1000,:], 'b')
ax[1,0].set_title('$t=$'+str(t[1000]))

ax[1,1].hist(particle_positions[1500,:],density=True)
ax[1,1].plot(x, c_exact[1500,:], 'k')
ax[1,1].set_title('$t=$'+str(t[1500]))

ax[0,0].set_xlim([-L/2,L/2])
ax[0,1].set_xlim([-L/2,L/2])
ax[1,0].set_xlim([-L/2,L/2])
ax[1,1].set_xlim([-L/2,L/2])
plt.xlabel('$x$')
plt.grid()
plt.show()
```

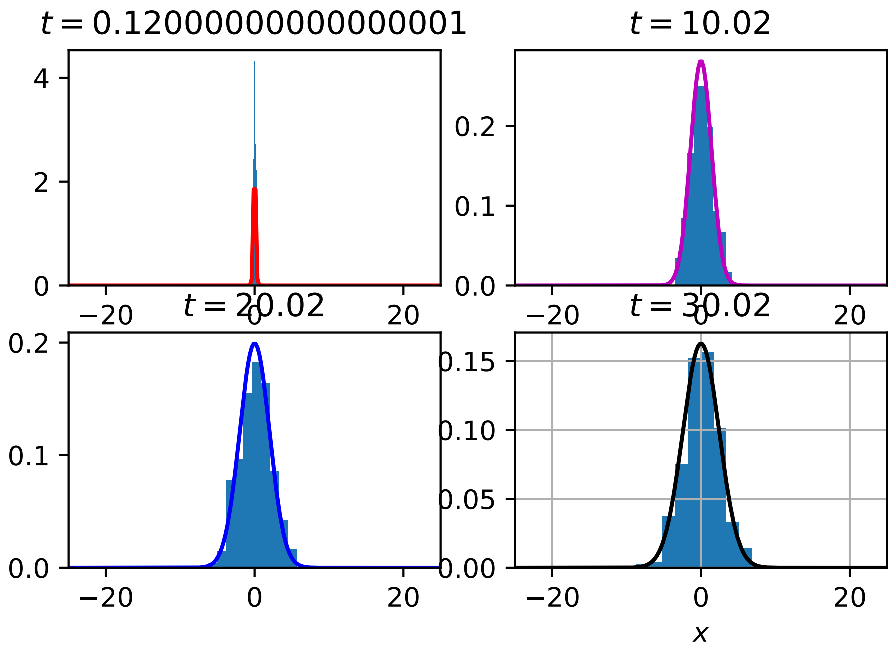

Figure 2.3: Numerical implementation of random walk

Concider 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

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

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 @#eq-fund_sol.

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

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

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

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

T=10
L=10

N_x=100
N_t=120

t=np.linspace(0,T,N_t)
x=np.linspace(0,L,N_x)-L/2

D=0.5
rho=1.0
epsilon=0.1

u_0=1/(epsilon*np.sqrt(np.pi))*np.exp(-x**2/epsilon**2)
```

```
dx=L/(N_x-1)
dt=T/(N_t-1)


def logisticPDErhs(u,t):
    N_x=len(u)
    f=np.zeros_like(u)
    for i in range(1,N_x-1):
      f[i]=D/dx**2*(u[i-1]-2*u[i]+u[i+1])


    i=0
    f[i]=D/dx**2*(-u[i]+u[i+1])
    i=N_x-1

    f[i]=D/dx**2*(u[i-1]-u[i])

    reac=rho*u
    f=f+reac
    return f

sol=odeint(logisticPDErhs,u_0,t)


[x_mesh,t_mesh]=np.meshgrid(x,t)

c_exact=1/np.sqrt(4*np.pi*D*t_mesh)*np.exp(rho*t_mesh-x_mesh**2/(4*D*t_mesh))

fig,ax=plt.subplots()
ax.plot(x, sol[1,:], 'r')
ax.plot(x, sol[4,:], 'b')
ax.plot(x, sol[8,:], 'm')
ax.plot(x, sol[12,:], 'k')
plt.legend(['t'+ str(t[0]),'t='+ str(t[4]),'t='+ str(t[8]),'t='+ str(t[12])])
plt.xlabel('$x$')
plt.grid()
plt.show()

fig,ax=plt.subplots()
ax.plot(x, c_exact[1,:], 'r')
ax.plot(x, c_exact[4,:], 'b')
```

```
ax.plot(x, c_exact[8,:], 'm')
ax.plot(x, c_exact[12,:], 'k')
plt.legend(['t'+ str(t[0]),'t='+ str(t[4]),'t='+ str(t[8]),'t='+ str(t[12])])
plt.xlabel('$x$')
plt.grid()
plt.show()
```

```
/var/folders/m_/vc0kz_0x6ls5n4qnksq052jw0000gp/T/ipykernel_21338/3455521560.py:46: RuntimeWa

divide by zero encountered in divide

/var/folders/m_/vc0kz_0x6ls5n4qnksq052jw0000gp/T/ipykernel_21338/3455521560.py:46: RuntimeWa

invalid value encountered in multiply
```

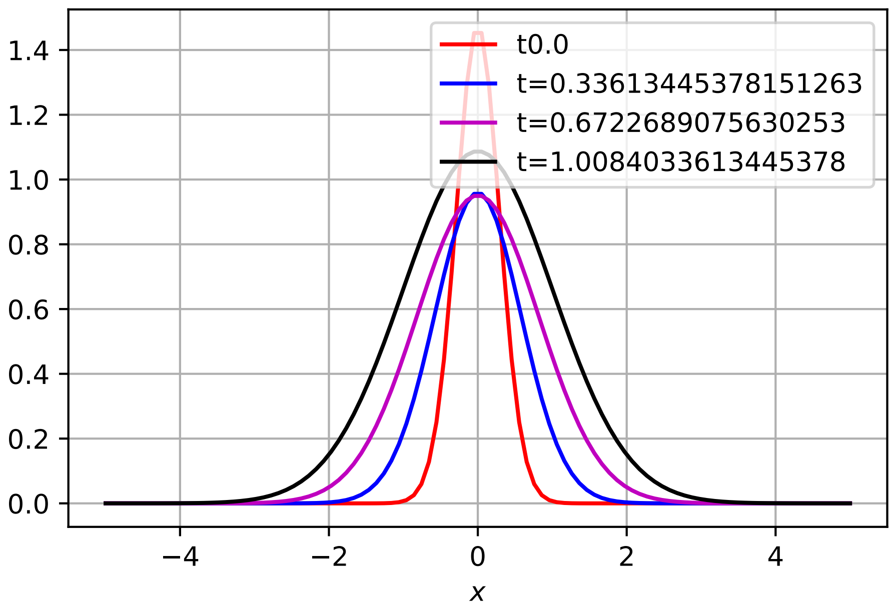

Figure 2.4: Numerical solution of linear reaction diffusion equation

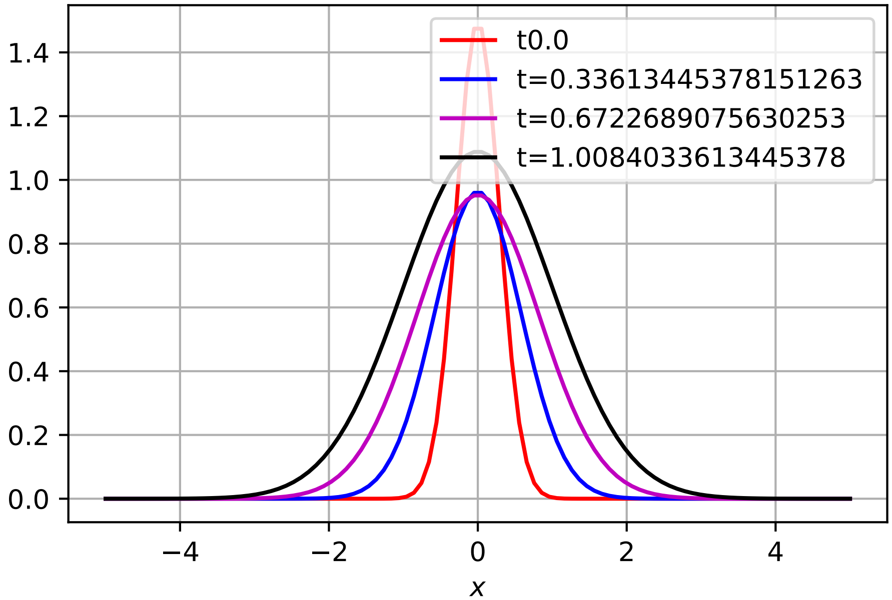

Figure 2.5: Exact solution of linear reaction diffusion equation

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

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

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 **??**,

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

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

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 $u \sim 0$.

- Can we prove this is a travelling wave (e.g. the solution could be dynamic on a very slow time scale that is not captured by the numeircal solution)?

- Can we derived a form for the travelling wave profile?
- Will we see a travelling wave for any initial data?
- How does the wave speed relate to model parameters?

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

T=100
L=100

N_x=100
N_t=100

t=np.linspace(1,T,N_t)
x=np.linspace(0,L,N_x)


u_0=0.5*(1+np.tanh(-0.1*(x-20)))

dx=L/(N_x-1)
dt=T/(N_t-1)


def logisticPDErhs(u,t):
    N_x=len(u)
    f=np.zeros_like(u)
    for i in range(1,N_x-1):
      f[i]=1/dx**2*(u[i-1]-2*u[i]+u[i+1])+u[i]*(1-u[i])


    i=0
    f[i]=1/dx**2*(-u[i]+u[i+1])+u[i]*(1-u[i])
    i=N_x-1

    f[i]=1/dx**2*(u[i-1]-u[i])+u[i]*(1-u[i])
    return f

sol=odeint(logisticPDErhs,u_0,t)

plt.plot(x, sol[0,:], 'r')
plt.plot(x, sol[4,:], 'b')
```

```
plt.plot(x, sol[8,:], 'm')
plt.plot(x, sol[12,:], 'k')
plt.legend(['t'+ str(t[0]),'t='+ str(t[4]),'t='+ str(t[8]),'t='+ str(t[12])])
plt.xlabel('$x$')
plt.grid()
plt.show()
```

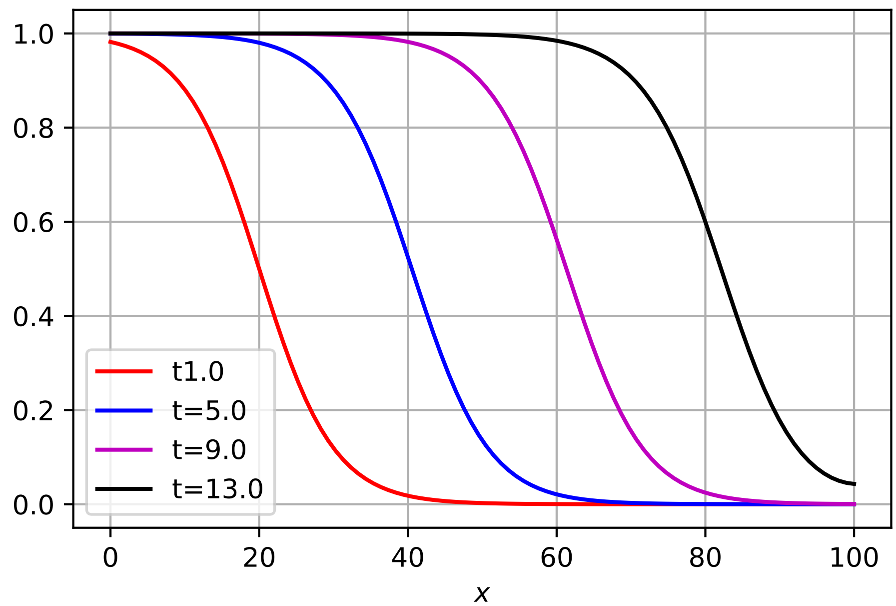

Figure 3.1: Numerical solution of Fisher's equation.

3.2 Travelling waves

It is known that the Fisher Equation **??** exhibits what are known as *travelling wave* solutions.

Definition 3.1. A travelling wave is a solution of a partial differential equation with a constant profile (shape) and a constant propagation speed.

3.2.1 Types of travelling waves

- Travelling pulse: $u(x,t) \to a$, as $x \to \pm\infty$.
- Travelling front : $u(x,t) \to a$, as $x \to -\infty$, $u(x,t) \to b$, as $x \to +\infty$ and $a \neq b$ (this is what we see in Figure **??**)

- Travelling train: $u(x,t)$ is a periodic function in x.

A travelling wave solution of a PDE can be written in the form $u(x,t) = W(z)$, where $z = x - vt$. We shall consider $v > 0$, which describes a wave moving from left to right.

Consider first the *spatially uniform (homogeneous)* solution of Equation **??**

$$\frac{\partial u}{\partial t} = u(1-u), \qquad t > 0. \tag{3.3}$$

Steady states of Equation **??** are

$$u = u_1 = 1$$

and

$$u = u_2 = 0.$$

To analyse the stability we consider

$$f(u) = u(1-u) \quad \text{and} \quad \frac{df}{du}(u) = 1 - 2u.$$

Then

$$\frac{df}{du}(u_1) = -1 \quad \text{and} \quad \frac{df}{du}(u_2) = 1.$$

Thus $u_1 = 1$ is *stable* and $u_2 = 0$ is *unstable*.

This stability analysis suggests that for the spatially dependent situation we can have a travelling wave solution that connects the two steady states u_1 and u_2 i.e. a travelling front.

Consider the travelling wave *ansatz*

$$u(x,t) = W(z) = W(x - vt),$$

where v is a constant. Changing variables in Equation **??** and using

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \frac{dW}{dz}\frac{\partial z}{\partial t} = -v\frac{dW}{dz}, \\
\frac{\partial u}{\partial x} &= \frac{dW}{dz}\frac{\partial z}{\partial x} = \frac{dW}{dz}, \\
\frac{\partial^2 u}{\partial x^2} &= \frac{d^2W}{dz^2}\left(\frac{\partial z}{\partial x}\right)^2 + \frac{dW}{dz}\frac{\partial^2 z}{\partial x^2} = \frac{d^2W}{dz^2},
\end{aligned}$$

we obtain a second order ordinary differential equation for W

$$\frac{d^2W}{dz^2} + v\frac{dW}{dz} + W(1-W) = 0, \tag{3.4}$$

where

$$W(z) \to 1 \quad \text{as} \quad z \to -\infty, \quad W(z) \to 0 \quad \text{as} \quad z \to +\infty, \tag{3.5}$$

and

$$W(z) \in [0, 1]. \tag{3.6}$$

We can rewrite Equation **??** as a system of two first order ODEs

$$\begin{aligned} \frac{dW}{dz} &= P = F(W, P), \\ \frac{dP}{dz} &= -vP - W(1 - W) = G(W, P). \end{aligned} \tag{3.7}$$

3.2.2 Numerical solutions

In Figure **??** we plot the numerical solution to equations Equation **??** for different values of the wavespeed, v. Note that when the wavespeed is too small the solution spirals in towards the origin. This solution cannot be valid as it implies that $u < 0$ for some z.

Note that some problem will not have a travelling wave solution. In this situation we could still make the travelling wave ansatz but this would usually result in a contradiction. In such a case this tells us that a travelling wave solution is not possible.

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

T=300

a=0.2
N_z=5000

z=np.linspace(1,T,N_z)

u_0=[0.99,-0.0001]

c_1=2.0
c_2=8.6
c_3=0.5

def fisherTrWaveODErhs(u, t, c):
    f=np.zeros_like(u)
    reaction=u[0]*(1-u[0])
```

```python
    f[0]=u[1]
    f[1]=-c*u[1]-reaction
    return f

sol=odeint(fisherTrWaveODErhs,u_0,z, args=(c_1,))
sol2=odeint(fisherTrWaveODErhs,u_0,z, args=(c_2,))
sol3=odeint(fisherTrWaveODErhs,u_0,z, args=(c_3,))

fig, ax = plt.subplots(1,2)
ax[0].plot(sol[:,0],sol[:,1], 'r')
ax[0].plot(sol2[:,0],sol2[:,1], 'b')
ax[0].plot(sol3[:,0],sol3[:,1], 'k')
ax[0].set_xlim([-0.5, 1.05])
ax[0].set_xlabel('$u$')
ax[0].set_ylabel('$du/dz$')

ax[1].plot(z,sol[:,0], 'r')
ax[1].plot(z,sol2[:,0], 'b')
ax[1].plot(z,sol3[:,0], 'k')
ax[1].set_xlim([-0.5, 100])

ax[1].set_xlabel('$z$')
ax[1].set_ylabel('$u$')
plt.legend(['c='+str(c_1),'c='+str(c_2), 'c='+str(c_3)])
plt.grid()
plt.show()
```

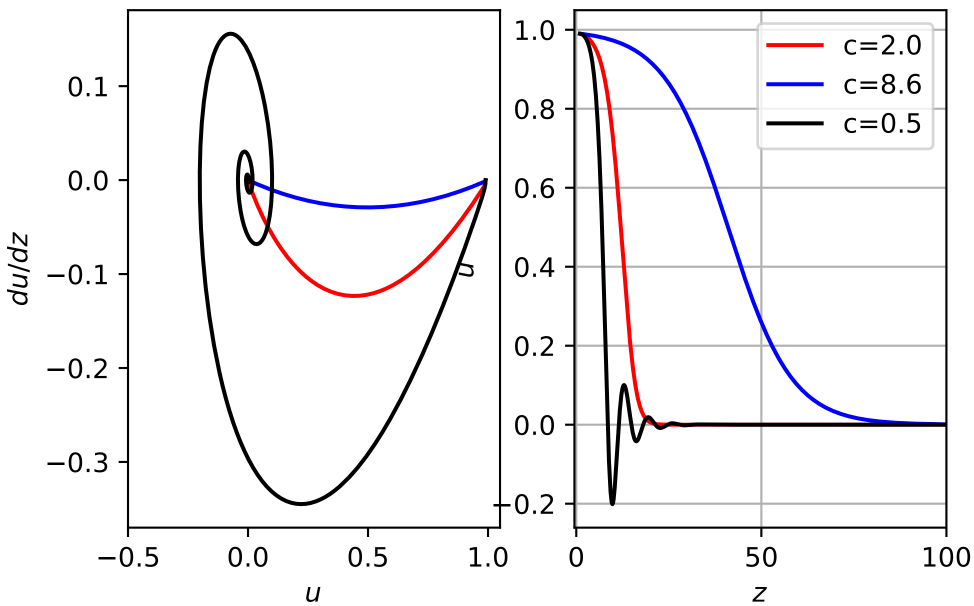

Figure 3.2: Proposed numerical solution of Equation **??** with prospective values of wavespeed c.

3.2.3 Steady state analysis

The steady states of Equation **??** are $(W_1, P_1) = (0, 0)$ and $(W_2, P_2) = (1, 0)$.

Using

$$\frac{dP}{dW} = \frac{dP}{dz}\frac{dz}{dW} = \frac{\frac{dP}{dz}}{\frac{dW}{dz}}$$

and Equation **??** we can write an equation for $P = P(W)$:

$$\frac{dP}{dW} = -v - \frac{W(1-W)}{P}, \tag{3.8}$$

together with

$$P(0) = 0, \quad P(1) = 0, \tag{3.9}$$

and

$$P(W) < 0 \quad \text{or} \quad W \in (0, 1). \tag{3.10}$$

The condition Equation **??** is given by the form of travelling front, which we would like to show that it exists

Lemma 3.1. *For every solution of Equation* **??** *satisfying Equation* **??** *and Equation* **??** *we have that* $\dfrac{dW(z)}{dz} < 0$ *for all finite* z*, i.e.*

$$P(W) < 0 \quad \text{for} \quad W \in (0,1).$$

Thus in phase-plane we shall look for a trajectory connecting $(W_1, P_1) = (0,0)$ and $(W_2, P_2) = (1,0)$ and $P < 0$.

3.2.4 Connection between sign of P and sign of speed v

Consider Equation **??**. Multiplying it by P and integrating over W from 0 to 1, we obtain

$$\int_0^1 \frac{dP}{dW} P(W)\, dW = -v \int_0^1 P(W) dW - \int_0^1 W(1-W) dW.$$

Using conditions Equation **??** we have

$$\int_0^1 \frac{dP}{dW}\, P\, dW = \frac{1}{2} \int \frac{d}{dW}(P^2) dW = \frac{1}{2}\left(P^2(1) - P^2(0)\right) = 0,$$

and

$$v \int_0^1 P(W) dW = -\int_0^1 W(1-W) dW < 0, \quad \text{since} \int_0^1 W(1-W) dW > 0.$$

Thus for $v > 0$ we have $P = W' < 0$ and for $v < 0$ we have $P = W' > 0$.

Note: $u(x,t) = W(z)$, where $z = x - vt$ with $v < 0$ and $\frac{dW}{dz} > 0$ will also be a travelling wave for the Fisher Equation **??**, i.e. a travelling wave front moving to the left.

Note: Instead of $z = x - vt$ we can also consider $z = x + vt$. The sign of v determines the direction of movement: If $z = x - vt$ for $v > 0$ we have travelling wave moving to the right and for $v < 0$ we have travelling wave moving to the left.

If $z = x + vt$ for $v > 0$ we have travelling wave moving to the left and for $v < 0$ we have travelling wave moving to the right.

3.2.5 Stability of steady states

The **Jacobian matrix** for Equation **??** is given by:

$$J(W,P) = \begin{pmatrix} \frac{\partial F}{\partial W} & \frac{\partial F}{\partial P} \\ \frac{\partial G}{\partial W} & \frac{\partial G}{\partial P} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 + 2W & -v \end{pmatrix}.$$

At $(W_1, P_1) = (0,0)$ the eigenvalues of $J(0,0)$ are solutions of the characteristic polynomial

$$\det(J(0,0) - \lambda I) = \begin{vmatrix} -\lambda & 1 \\ -1 & -v-\lambda \end{vmatrix} = \lambda^2 + v\lambda + 1 = 0.$$

Thus

$$\lambda_1^{\pm} = \frac{1}{2}(-v \pm \sqrt{v^2 - 4})$$

and we have for $v > 0$ that $Re(\lambda_1^{\pm}) < 0$.

Therefore at $(0,0)$

$$\begin{cases} \text{stable node if } v^2 \geq 4, \\ \text{stable focus if } v^2 \leq 4 \quad (\text{ complex eigenvalues}) \end{cases}$$

At $(W_2, P_2) = (1,0)$ the eigenvalues of $J(1,0)$ are solutions of the characteristic polynomial

$$\det(J(1,0) - \lambda I) = \begin{vmatrix} -\lambda & 1 \\ 1 & -v-\lambda \end{vmatrix} = \lambda^2 + v\lambda - 1 = 0.$$

Thus

$$\lambda_2^{\pm} = \frac{1}{2}(-v \pm \sqrt{v^2 + 4})$$

and we have for $v > 0$ that $\lambda_2^- < 0 < \lambda_2^+$. Therefore $(1,0)$ is a saddle.

The eigenvectors are defined by

$$-\lambda W + P = 0.$$

Thus at $(W_1, P_1) = (0,0)$ we have

$$\Phi_1 = \begin{pmatrix} W \\ \lambda_1^- W \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} W \\ \lambda_1^+ W \end{pmatrix}.$$

Consider that

$$\lambda_1^- \leq \lambda_1^+ < 0 \quad \text{and choose} \quad W = \pm 1.$$

At $(W_2, P_2) = (1,0)$ we have

$$\Psi_1 = \begin{pmatrix} W \\ \lambda_2^- W \end{pmatrix}, \quad \Psi_2 = \begin{pmatrix} W \\ \lambda_2^+ W \end{pmatrix}.$$

Consider that

$$\lambda_2^- < 0 < \lambda_2^+ \quad \text{and choose} \quad W = \pm 1.$$

The eigenvectors are sketched in Figure **??**.

Definition 3.2. The trajectory that connects two different points is called a heteroclinic connection. The trajectory that connects a point with itself is called a homoclinic connection.

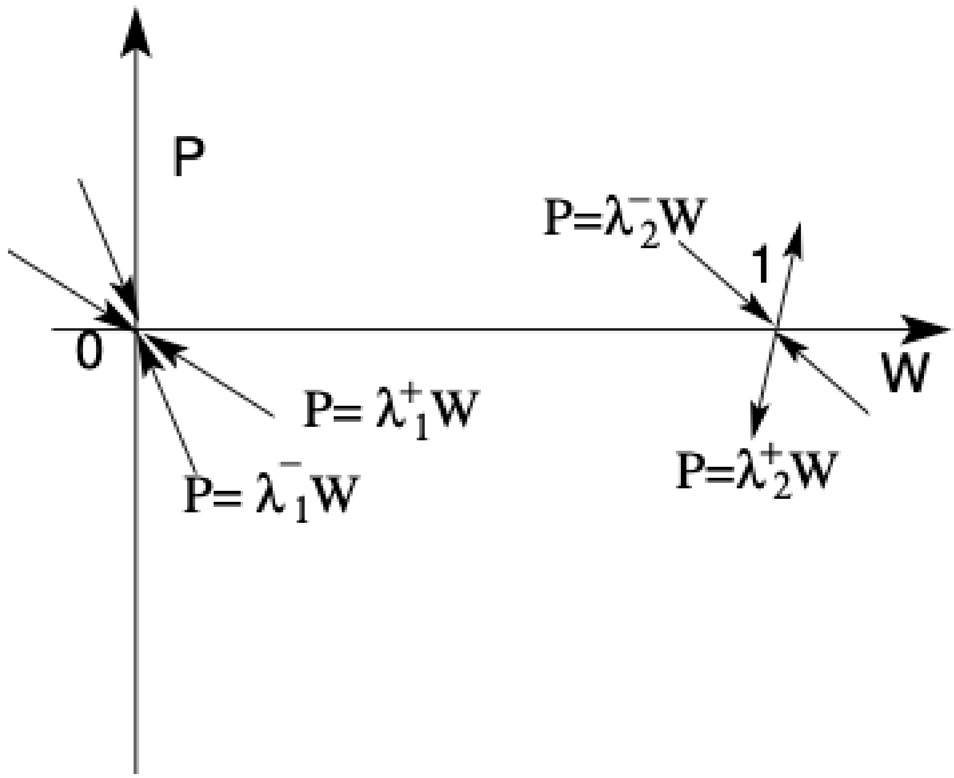

Figure 3.3: Schematic diagram of eigenvectors.

3.2.6 Minimal wave speed

It can be shown that for $v < 2$ a heteroclinic connection between $(0, 0)$ and $(1, 0)$ exists, but in this situation the steady state $(0, 0)$ is a stable focus and corresponds to an oscillatory front.

In the context of a model of a biological process W is the profile of a population density and $W \geq 0$. Hence, for $v < 2$ trajectories connecting $(0, 0)$ and $(1, 0)$ are not biologically realistic.

Thus we obtain the minimal speed $v^*_{\min} = 2$ (non-dimensionalized) for which we have a travelling wave front solution for Fisher's equation.

In the original dimensional variables we have:

$$z^* = x^* - v^* t^* = x\sqrt{\frac{\rho}{D}} - v^* t\rho, \quad \sqrt{\frac{D}{\rho}} z^* = x - \sqrt{D\rho}\, v^*\, t.$$

Thus for $z = x - vt$ we have

$$v = v^* \sqrt{D\rho},$$

and

$$v_{\min} = v^*_{\min}\sqrt{D\rho} = 2\sqrt{D\rho}.$$

3.2.6.1 The existence of a confined region

To show the existence of a travelling wave we will construct a **confined region** or **confined set** in $\mathbb{R}^2$, which contains both steady states such that, once inside this region solution trajectories cannot escape from it (also known as an **invariant region** or **invariant set**).

Consider

$$T = \{(W, P) : 0 \leq W \leq 1,\ P \leq 0,\ P \geq \mu W\}$$

for some $\mu < 0$.

Consider normal vectors at each boundary of T:

$$\text{at } P = 0 \ :\ n_1 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \quad \text{at } W = 1 \ :\ n_2 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}, \quad \text{at } P = \mu W \ :\ n_3 = \begin{pmatrix} -\mu \\ 1 \end{pmatrix}.$$

Consider the scalar product between normal vectors and the **flow vector**

$$\begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix},$$

of Equation **??**.

At $P = 0$

$$\begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot n_1 = \begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot \begin{pmatrix} 0 \\ -1 \end{pmatrix} = (vP + W(1-W))\Big|_{P=0} = W(1-W) \geq 0, \text{ for } W \in [0,1].$$

At $W = 1$

$$\begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot n_2 = \begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot \begin{pmatrix} -1 \\ 0 \end{pmatrix} = -P \geq 0, \text{ since } P \leq 0.$$

At $P = \mu W$

$$\begin{aligned} \begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot n_3 &= \begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot \begin{pmatrix} -\mu \\ 1 \end{pmatrix} \\ &= (-\mu P - vP - W(1-W))\Big|_{P=\mu W} \\ &= -\mu^2 W - \mu v W - W(1-W) = -W(\mu^2 + \mu v + 1) + W^2. \end{aligned}$$

Thus

$$\begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot n_3 \geq 0,$$

if

$$\mu^2 + \mu v + 1 \leq 0.$$

The last inequality is satisfied if we have real roots of the equation $\mu^2 + \mu v + 1 = 0$. We have that

$$\mu_{1,2} = \frac{-v \pm \sqrt{v^2 - 4}}{2}$$

are real if $v^2 \geq 4$.

Thus, since $v > 0$, for $v \geq 2$ and any

$$\mu \in \left[\frac{-v - \sqrt{v^2 - 4}}{2}, \frac{-v + \sqrt{v^2 - 4}}{2} \right]$$

we have

$$\begin{pmatrix} \dfrac{dW}{dz} \\ \\ \dfrac{dP}{dz} \end{pmatrix} \cdot n_3 \geq 0 \qquad \text{at} \quad P = \mu W.$$

Therefore we have shown that at the boundaries of T the flow vector points in to the region T and any trajectory approaching the boundaries from inside of T will return to T without crossing any of the boundaries of T. Thus we have constructed an invariant (trapping) triangular region containing the steady states $(0, 0)$ and $(1, 0)$.

If we can show that there no other steady states or periodic solutions of the system Equation **??**, then a trajectory that leaves $(1, 0)$ must approach $(0, 0)$.

Theorem 3.1. *Bendixson's Negative Criterion, Dulac's Negative Criterion*

If there exists a function $\varphi(W, P)$, with $\varphi \in C^1(\mathbb{R}^2)$, such that

$$\frac{\partial(\varphi F)}{\partial W} + \frac{\partial(\varphi G)}{\partial P},$$

has the same sign ($\neq 0$) almost everywhere in a simply connected region (region without holes), then the system

$$\frac{dW}{dz} = F(W, P) \ ,$$
$$\frac{dP}{dz} = G(W, P),$$

has no periodic solutions in this region.

We can apply Theorem **??** to our situation taking $\varphi(W, P) = 1$. Then using Equation **??** we have

$$\frac{\partial(\varphi F)}{\partial W} + \frac{\partial(\varphi G)}{\partial P} = -v < 0 \ .$$

Thus we have no periodic solutions and also only two steady states $(0, 0)$ and $(1, 0)$ in the confined (invariant) simply-connected region T. Therefore the trajectory that leaves $(1, 0)$ will approach $(0, 0)$.

We have therefore shown that for any $v \geq 2$ there exist a heteroclinic trajectory $P(W)$ connecting $(0, 0)$ and $(1, 0)$.

Theorem 3.2. *For $P(W)$ satisfying Equation **??**, Equation **??** and $P(W) < 0$ for $W \in (0, 1)$, there exists a solution $W(z)$ of Equation **??** satisfying Equation **??** and Equation **??**.*

Thus for any wave speed v satisfying $v \geq 2$, we have the existence of travelling wave front $u(x, t) = W(x - vt)$ of Fisher's equation Equation **??**.

3.2.7 Initial conditions

One final key question is: For which initial conditions $u(x, 0) = u_0(x)$ does the solution evolve to a travelling wave solution?

If we start with a travelling wave shape initial condition, i.e. $u_0(x) = W(z)|_{t=0} = W(x)$, then this simply propagates as a travelling wave. However if $u_0(x) \neq W(x)$, then it is not immediately obvious how the solution will evolve. This problem was considered by Kolmogorov et al. Kolmogorov, Petrovsky, and Piskunov (1937), who showed that for any initial data satisfying

$$u_0(x) \geq 0, \quad \text{with} \quad u_0(x) = \begin{cases} 1 & \text{if } x \leq x_1, \\ 0 & \text{if } x \geq x_2, \end{cases}$$

where $x_1 < x_2$ and u_0 is continuous in $[x_1, x_2]$, the solution of Fisher's Equation **??** evolves to a travelling wave with minimal speed

$$v_{\text{min}} = 2\sqrt{\rho D}$$

and

$$u(t, x) \to 1 \quad \text{as} \quad x \to -\infty, \quad u(t, x) \to 0 \quad \text{and} \quad x \to +\infty.$$

3.3 Travelling waves in bistable equations

Consider now the reaction-diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(u) \qquad x \in \mathbb{R},\ t > 0, \tag{3.11}$$

with initial condition

$$u(x, 0) = u_0(x) \qquad x \in \mathbb{R},$$

where $f(0) = f(a) = f(1) = 0$ and $0 < a < 1$. There are three spatially uniform steady states $u_1 = 0$, $u_2 = a$, $u_3 = 1$.

The stability of the steady states is given by the sign of $f'(u_j)$ for $j = 1, 2, 3$.

If we have that $f'(0) < 0$, $f'(a) > 0$ and $f'(1) < 0$ then $u_1 = 0$ and $u_3 = 1$ are stable steady states and $u_2 = a$ is an unstable steady state of Equation **??**.

An example of such a function is f is $f = u(u - a)(1 - u)$ which arises in the study of nerve action potentials along nerve fibres and other problems in **excitable media**.

The existence of two stable steady states gives rise to the name "bistable equation'".

3.4 Numerical solutions

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

T=100
L=100

a=0.2

N_x=100
N_t=100

t=np.linspace(1,T,N_t)
x=np.linspace(0,L,N_x)


u_0=6*0.5*(1+np.tanh(-1*(x-50)))*0.5*(1+np.tanh(1*(x-50)))
u_0=0.5*(1+np.tanh(-1*0.2*(x-50)))

dx=L/(N_x-1)
dt=T/(N_t-1)

fig, ax = plt.subplots(1)
u_samp=np.linspace(0,1,100)
reac=u_samp*(u_samp-a)*(1-u_samp)
ax.plot(u_samp,reac)
ax.set_xlabel('$u$')
ax.set_ylabel('$f(u)$')

plt.show()


def bistablePDErhs(u,t):
    N_x=len(u)
    f=np.zeros_like(u)
    for i in range(1,N_x-1):
      f[i]=1/dx**2*(u[i-1]-2*u[i]+u[i+1])
    i=0
    f[i]=1/dx**2*(-u[i]+u[i+1])
```

```
    i=N_x-1

    f[i]=1/dx**2*(u[i-1]-u[i])

    reaction=u*(u-a)*(1-u)
    f= f+reaction
    return f

sol=odeint(bistablePDErhs,u_0,t)

plt.plot(x, sol[0,:], 'r')
plt.plot(x, sol[15,:], 'b')
plt.plot(x, sol[30,:], 'm')
plt.plot(x, sol[45,:], 'k')
plt.legend(['t'+ str(t[0]),'t='+ str(t[4]),'t='+ str(t[8]),'t='+ str(t[12])])
plt.xlabel('$x$')
plt.grid()
plt.show()
```

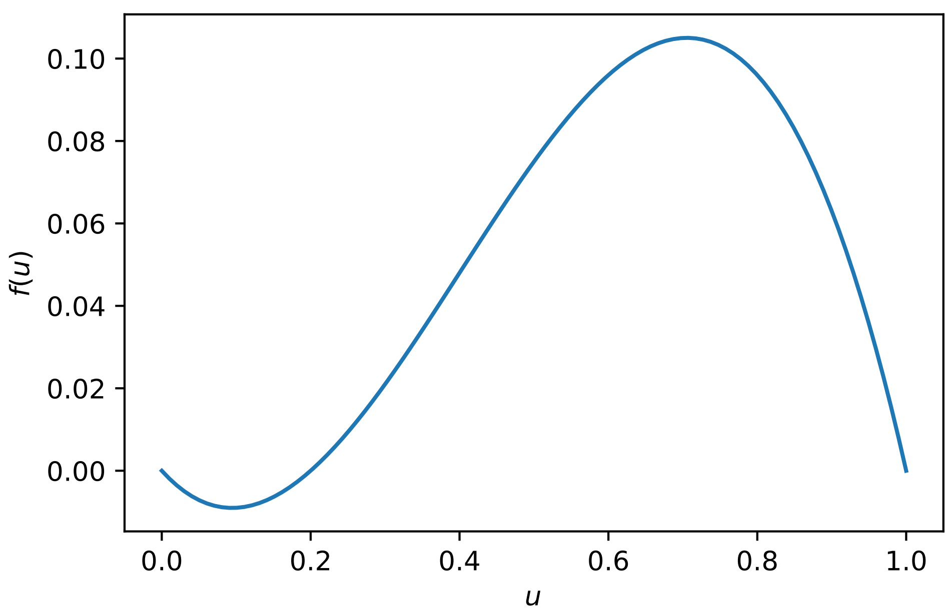

Figure 3.4: A plot of f(u) against u.

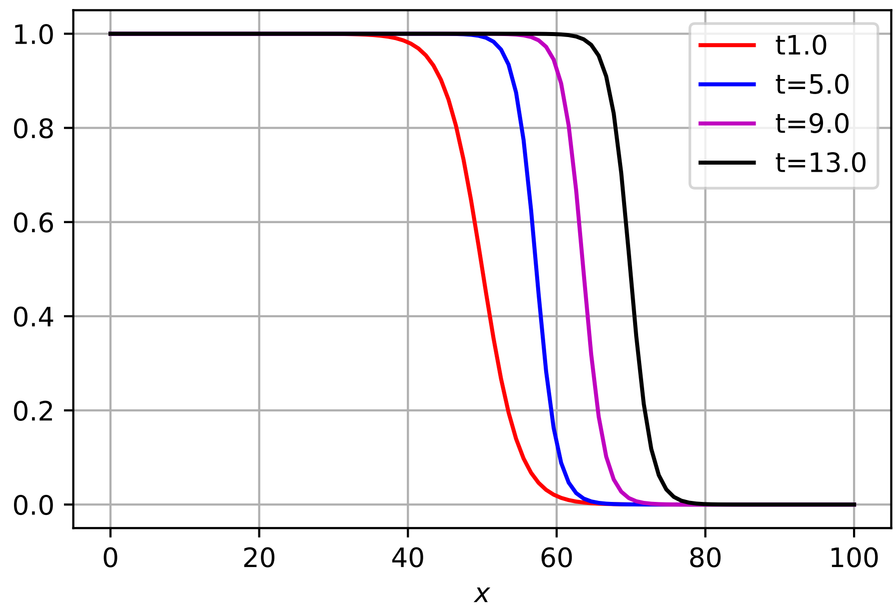

Figure 3.5: Numerical solution of bistable PDE.

3.5 General assumptions on f

- $f(0) = f(a) = f(1) = 0,$
- $f(u) < 0$ in $(0, a)$, $\quad f(u) > 0$ in $(a, 1)$
- $f'(0) < 0, \quad f'(1) < 0$

In a similar manner to the previous sections, we look for a travelling wave solution of the form $u(x,t) = W(z)$ with $z = x - vt$, yielding

$$\frac{d^2W}{dz^2} + v\frac{dW}{dz} + f(W) = 0, \ . \tag{3.12}$$

We can rewrite Equation **??** as asystem of two 1st order ODEs

$$\begin{aligned} \frac{dW}{dz} &= P = F(W,P), \\ \frac{dP}{dz} &= -vP - f(W) = G(W,P), \end{aligned} \tag{3.13}$$

3.5.1 Stability of the steady states

The steady states of Equation **??** are $(W_1, P_1) = (0, 0)$, $(W_2, P_2) = (a, 0)$, $(W_3, P_3) = (1, 0)$.

The Jacobian matrix is given by

$$J(W, P) = \begin{pmatrix} \frac{\partial F}{\partial W} & \frac{\partial F}{\partial P} \\ \frac{\partial G}{\partial W} & \frac{\partial G}{\partial P} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -f'(W) & -v \end{pmatrix}$$

At steady states (W_j, P_j), the eigenvalues of $J(W_j, P_j)$ are solutions of the characteristic polynomial

$$\det(J(W_j, P_j) - \lambda I) = \begin{vmatrix} -\lambda & 1 \\ -f'(W_j) & -v - \lambda \end{vmatrix} = \lambda^2 + v\lambda + f'(W_j) = 0.$$

Therefore:

$$\lambda_j^{\pm} = \frac{-v \pm \sqrt{v^2 - 4f'(W_j)}}{2}.$$

At $(W_1, P_1) = (0, 0)$ since $f'(0) < 0$ we obtain $ _1^{-} <0< _1^{+} $ and it is a saddle point. \

At $(W_2, P_2) = (a, 0)$ since $f'(a) > 0$ we obtain

$$(a, 0) - \begin{cases} \text{focus} & \text{if } v^2 < 4f'(a) \text{ and is stable if } v > 0, \text{ unstable if } v < 0, \\ \text{node} & \text{if } v^2 \geq 4f'(a) \text{ and is stable if } v > 0, \text{ unstable if } v < 0, \\ \text{centre} & \text{if } v = 0\ . \end{cases}$$

\ At $(W_3, P_3) = (1, 0)$ since $f'(1) < 0$ we obtain $ _3^{-} <0< _3^{+} $ and it is a saddle point. \

Eigenvectors are given by

$$P = \lambda W$$

and at each steady state we have two eigenvectors

$$\Psi_j^{\pm} = \begin{pmatrix} W \\ \lambda_j^{\pm} W \end{pmatrix}, \qquad j = 1, 2, 3.$$

As we vary the wave speed v, the stable and unstable manifolds move and we wish to show that for some v the unstable manifold leaving one saddle point coincides with the stable manifold entering the other saddle point, i.e. we can choose a value for the wave speed v such that a heteroclinic connection between $(1, 0)$ and $(0, 0)$ is obtained. We shall use a “shooting argument” to prove this.

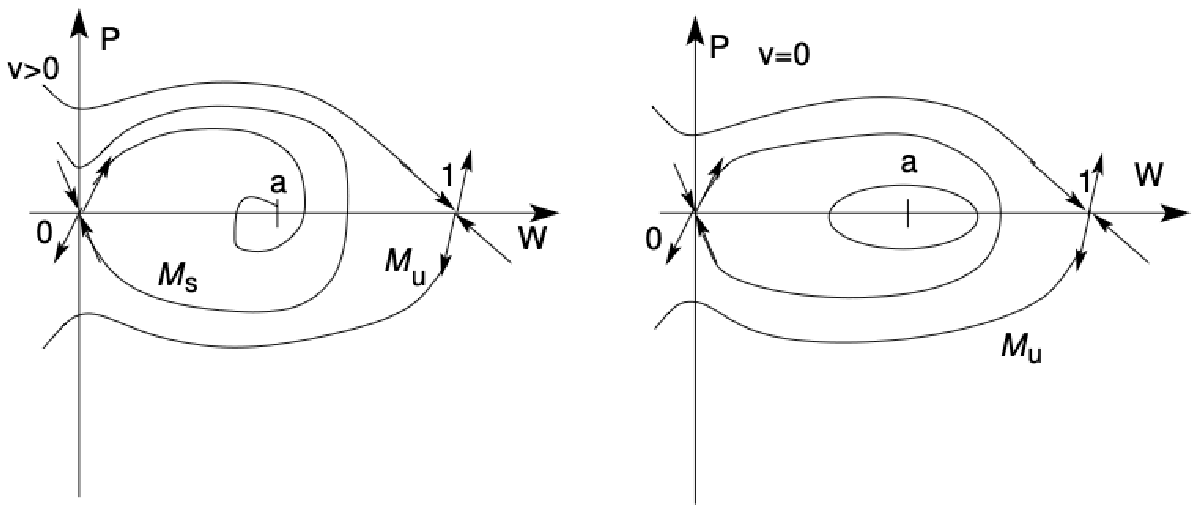

Figure 3.6: Schematic diagram of eigenvectors.

3.5.2 Relation between sign of v and sign of $\int\limits_0^1 f(u)\,du$

Consider Equation **??**, multiply it by $\dfrac{dW}{dz}$ and integrate over $(-\infty, +\infty)$:

$$\int_{-\infty}^{+\infty} \frac{d^2W}{dz^2}\frac{dW}{dz}\,dz + v\int_{-\infty}^{+\infty}\left|\frac{dW}{dz}\right|^2 dz + \int_{-\infty}^{+\infty} f(W)\frac{dW}{dz}\,dz = 0.$$

Then

$$\frac{1}{2}\int_{-\infty}^{+\infty}\frac{d}{dz}\left(\left|\frac{dW}{dz}\right|^2\right)dz + v\int_{-\infty}^{+\infty}\left|\frac{dW}{dz}\right|^2 dz + \int_{W(-\infty)}^{W(+\infty)} f(W)\,dW = 0$$

and since $W(z) \to 1$ as $z \to -\infty$ and $W(z) \to 0$ as $z \to +\infty$ we obtain

$$\frac{1}{2}\left(\left|\frac{dW(+\infty)}{dz}\right|^2 - \left|\frac{dW(-\infty)}{dz}\right|^2\right) + v\int_{-\infty}^{+\infty}\left|\frac{dW}{dz}\right|^2 dz + \int_1^0 f(W)\,dW = 0.$$

The fact that W is constant at $\pm\infty$ implies that

$$\frac{dW}{dz}\Big|_{z=-\infty} = \frac{dW}{dz}\Big|_{z=+\infty} = 0.$$

Thus we have

$$v\int\limits_{-\infty}^{+\infty}\left|\frac{dW}{dz}\right|^2 dz = \int\limits_0^1 f(W)dW$$

and

$$v = \frac{\int\limits_0^1 f(W)\,dW}{\int\limits_{-\infty}^{+\infty} \left|\frac{dW}{dz}\right|^2 dz}.$$

Since $\int\limits_{-\infty}^{+\infty} \left|\frac{dW}{dz}\right|^2 dz > 0$ we can conclude that

$$\int_0^1 f(u)\,du > 0 \quad \Longrightarrow \quad v > 0, \int_0^1 f(u)\,du = 0 \quad \Longrightarrow \quad v = 0, \int_0^1 f(u)\,du < 0 \quad \Longrightarrow \quad v < 0.$$

3.5.3 The shooting method proof of a heteroclinic connection

3.5.3.1 Numerical shooting method

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

T=300

a=0.2
N_z=5000

z=np.linspace(1,T,N_z)

u_0=[0.99,-0.0001]

c_1=2.0
c_2=0.6
c_3=0.425

def bistableTrWaveODErhs(u, t, c):
    f=np.zeros_like(u)
    reaction=u[0]*(u[0]-a)*(1-u[0])

    f[0]=u[1]
    f[1]=-c*u[1]-reaction
    return f
```

```
sol=odeint(bistableTrWaveODErhs,u_0,z, args=(c_1,))
sol2=odeint(bistableTrWaveODErhs,u_0,z, args=(c_2,))
sol3=odeint(bistableTrWaveODErhs,u_0,z, args=(c_3,))

fig, ax = plt.subplots(1)
plt.plot(sol[:,0],sol[:,1], 'r')
plt.plot(sol2[:,0],sol2[:,1], 'b')
plt.plot(sol3[:,0],sol3[:,1], 'k')
ax.set_xlim([-0.05, 1.05])

plt.xlabel('$u$')
plt.ylabel('$du/dz$')
plt.legend(['c='+str(c_1),'c='+str(c_2), 'c='+str(c_3)])
plt.grid()
plt.show()
```

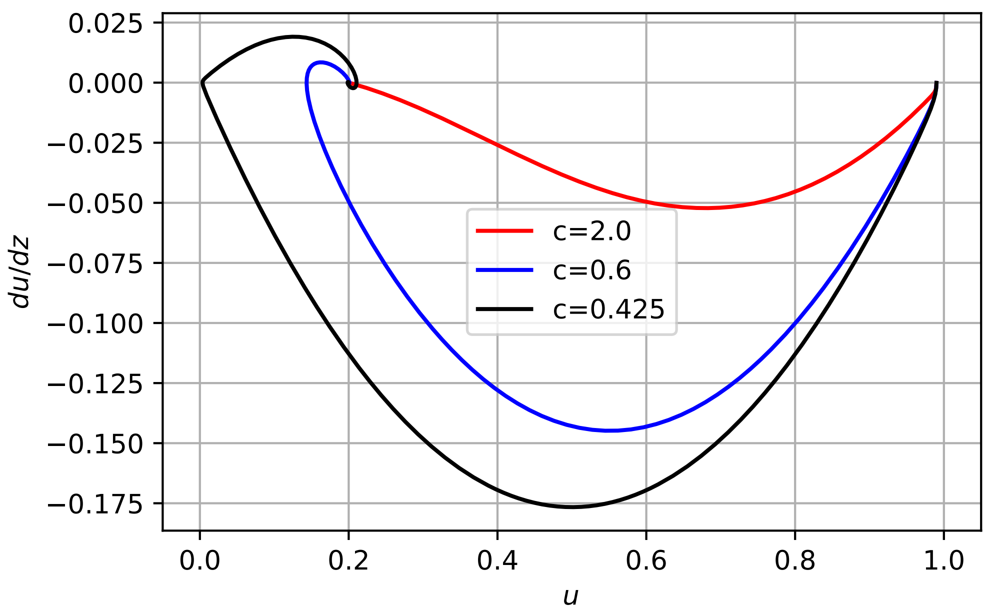

Figure 3.7: Numerical solution of bistable PDE

Assume

$$\int_0^1 f(u)\,du > 0.$$

i.e. $v > 0$.

- Consider first $v = 0$.

  From the equations in Equation **??** and the assumptions on the function f we have

  - If $W \in (0, a)$

    Using the fact that $f(W) < 0$ for $W \in (0, a)$ and $P < 0$ and $v = 0$ we have

    $$\begin{cases} \dfrac{dW}{dz} = P < 0, \\ \dfrac{dP}{dz} = -f(W) > 0 \end{cases} \qquad \rightarrow \qquad \frac{dP}{dW} < 0$$

    Thus the trajectory enters $(0, 0)$ with

    $$\frac{dP}{dW} < 0,$$

    along the stable manifold $M_s^{(0,0)}$ and intersects the line $\{W = a\}$ at the point (a, P_0).

  - If $W \in (a, 1)$

    Using the fact that $f(W) > 0$ for $W \in (a, 1)$ and $P < 0$ and $v = 0$ we have

    $$\begin{cases} \dfrac{dW}{dz} = P < 0, \\ \dfrac{dP}{dz} = -f(W) < 0 \end{cases} \qquad \rightarrow \qquad \frac{dP}{dW} > 0$$

    Thus the trajectory leaves $(1, 0)$ with

    $$\frac{dP}{dW} > 0$$

    along the unstable manifold $M_u^{(1,0)}$ and intersects the line $\{W = a\}$ at the point (a, P_1).

Now we shall compare P_0 and P_1. For this we consider again equation Equation **??**, multiply by $\dfrac{dW}{dz}$ and integrate first over $(-\infty, z^*)$ and then over $(z^*, +\infty)$, where $z^* \in (-\infty, +\infty)$ such that $W(z^*) = a$. Then since $v = 0$ we have first

$$\int_{-\infty}^{z^*} \frac{d^2W}{dz^2} \frac{dW}{dz}\, dz + \int_{-\infty}^{z^*} f(W) \frac{dW}{dz}\, dz = 0.$$

and

$$\frac{1}{2} \left| \frac{dW}{dz} \right|^2 \Big|_{z=-\infty}^{z=z^*} + \int_{W(-\infty)}^{W(z^*)} f(W) dW = 0\ .$$

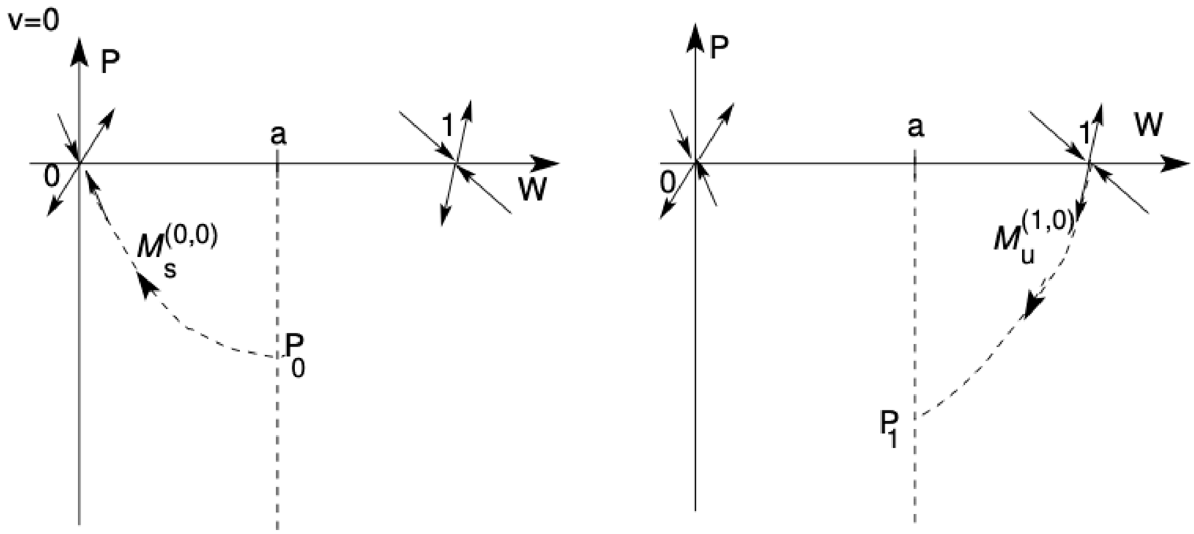

Figure 3.8: Schematic diagram of eigenvectors.

Since $W(-\infty) = 1$ we are moving along the unstable manifold $M_u^{(1,0)}$ and

$$\frac{dW(z^*)}{dz} = P(z^* + 0) = P_1.$$

Thus using that $\frac{dW}{dz}\Big|_{z=-\infty} = 0$ we obtain

$$\frac{1}{2}P_1^2 + \int_1^a f(W)dW = 0 \quad \Longrightarrow \quad P_1^2 = 2\int_a^1 f(W)dW$$

Integration over $(z^*, +\infty)$ implies

$$\int_{z^*}^{+\infty} \frac{d^2W}{dz^2}\frac{dW}{dz}\, dz + \int_{z^*}^{+\infty} f(W)\frac{dW}{dz}\, dz = 0.$$

and

$$\frac{1}{2}\left|\frac{dW(+\infty)}{dz}\right|^2 - \frac{1}{2}\left|\frac{dW(z^*)}{dz}\right|^2 + \int_{W(z^*)}^{W(+\infty)} f(W)\, dW = 0\ .$$

Since $W(+\infty) = 0$ we are moving along the stable manifold $M_s^{(0,0)}$ and $\frac{dW(z^*)}{dz} = P(z^* - 0) = P_0$. Thus using that $\frac{dW}{dz}\Big|_{z=+\infty} = 0$ we obtain

$$-\frac{1}{2}P_0^2 + \int_a^0 f(W)dW = 0 \quad \Longrightarrow \quad P_0^2 = -2\int_0^a f(W)dW\ .$$

Since

$$\int_0^1 f(u)\,du > 0$$

we obtain

$$P_1^2 - P_0^2 = 2\int_0^1 f(W)\,dW > 0 \quad \Longrightarrow \quad P_1^2 > P_0^2$$

Then since $P < 0$ we have

$$P_1 < P_0 \,.$$

- Consider $v > 0$ large.

From the equations in Equation **??** and the assumptions on the function f we have

```
* If $W \in (0,a)$
```

Using the fact that $f(W) < 0$ for $W \in (0, a)$, $P < 0$ and $v > 0$ we have

$$\begin{cases} \dfrac{dW}{dz} &= P < 0, \\ \dfrac{dP}{dz} &= -vP - f(W) > 0 \end{cases} \quad \Longrightarrow \quad \frac{dP}{dW} < 0$$

Thus $P(W)$ is always decreasing for $W \in (0, a)$. * If $W \in (a, 1)$

Using the fact that $f(W) > 0$ for $W \in (a, 1)$, $P < 0$ and $v > 0$ we have

$$\frac{dW}{dz} = P < 0,$$

$$\begin{cases} \dfrac{dP}{dz} = -vP - f(W) < 0 \quad \text{for small } |P| \text{ and } \dfrac{dP}{dz} = -vP - f(W) > 0 \quad \text{for large } |P|. \end{cases}$$

Thus

$$\begin{cases} \dfrac{dP}{dW} > 0 & \text{for small } |P|, \\ \\ \dfrac{dP}{dW} < 0 & \text{for large } |P| \,. \end{cases}$$

Therefore if $v > 0$ large we have that $P(W)$ is monotone increasing for small $|P|$ and monotone decreasing for large $|P|$.

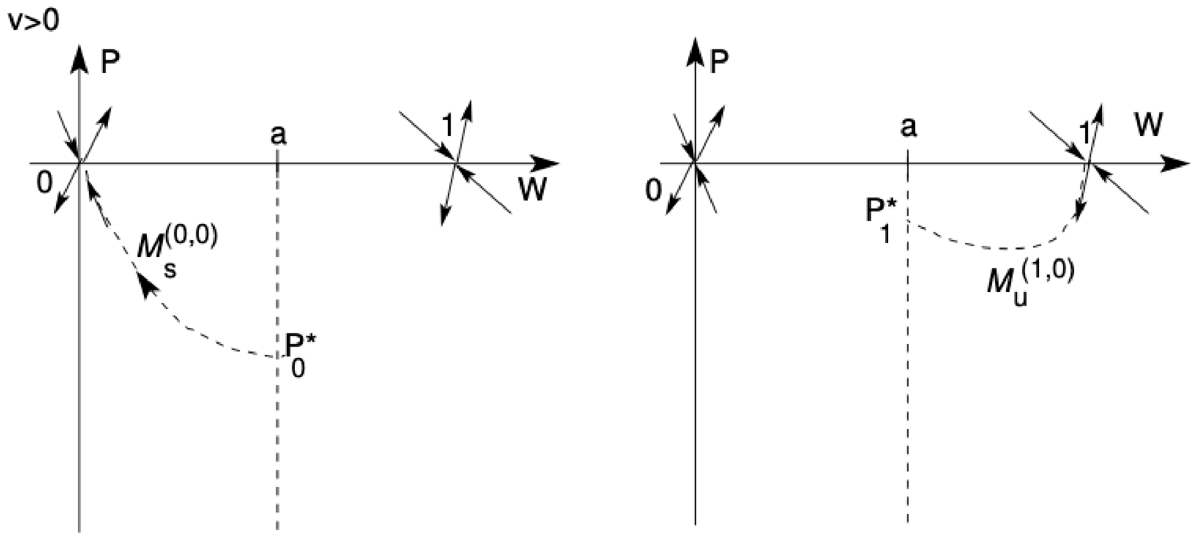

Figure 3.9: Schematic diagram.

Thus since for $v = 0$ we have $P_1 < P_0$ and for $v > 0$ we have that $P(W)$ is monotone decreasing for large $|P|$, due to the continuity of the phase trajectories with respect to the velocity v we obtain that there exists a travelling wave speed $v_0 > 0$ such that $P_0 = P_1$ and we have a heteroclinic connection between $(1, 0)$ and $(0, 0)$ in the phase plane. Hence for $v = v_0$ there exists a travelling wave front solution for the bistable Equation **??**.

We can repeat the analysis for

$$\int_0^1 f(u)\, du < 0$$

and obtain a travelling wave solution with $v_0 < 0$.

If

$$\int_0^1 f(u)\, du = 0,$$

then we have a standing wave with $v = 0$, since the calculations for P_0 and P_1 implies $P_0 = P_1$ and there exists a heteroclinic orbit between $(1, 0)$ and $(0, 0)$ in the phase space.

Note: There exists a unique travelling wave velocity v for which we have a travelling wave solution for bistable Equation **??**.

3.6 References

Part II

Multi species

4 Lotka Voltera model

Consider a predator-prey system (modified Lotka-Voltera equations) with diffusion of both the prey and the predator species. Suppose that the reaction kinetics are given by:

- prey undergoes logistic growth in the absence of predator.
- the predation rate is proportional to the amount of predator
- predator growth rate is proportional to the amount of prey
- predator undergoes natural degradation

Suppose also that both predator and prey undero random motion.

Let $u(x,t)$ and $n(x,t)$ represent the density of the prey and predator, respectively. The governing equations are:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \rho\, u \left(1 - \frac{u}{K}\right) - \alpha\, u\, n + D_u \Delta u, \\ \frac{\partial n}{\partial t} &= \beta\, u\, n - \gamma\, n + D_n \Delta n, \end{aligned} \tag{4.1}$$

where

- ρ – prey growth rate,
- K – carrying capacity,
- βu – growth rate of the predator,
- α – rate at which the predator eats the prey,
- γ – death rate of the predator,
- D_u – diffusion coefficient of the prey
- D_n - diffusion coefficient for the predator .

We will consider one spatial dimension.

4.1 Nondimensionalization

Consider the scaling

$$x^* = x\sqrt{\frac{\rho}{D_n}}, \qquad t^* = \rho, t, \quad u^* = \frac{u}{K}, \quad n^* = n\frac{\alpha}{\rho}.$$

Upon dropping the asteriked notation, Equation **??** transform to

$$\begin{cases} \dfrac{\partial u}{\partial t} = u(1-u-n) + D\dfrac{\partial^2 u}{\partial x^2} \; = \; f(u,n) + D\dfrac{\partial^2 u}{\partial x^2} \qquad x \in \mathbb{R}, t > 0\,, \\ \dfrac{\partial n}{\partial t} = a\,n(u-b) + \dfrac{\partial^2 n}{\partial x^2} \; = \; g(u,n) + \dfrac{\partial^2 n}{\partial x^2} \qquad x \in \mathbb{R}, t > 0, \end{cases} \tag{4.2}$$

where

$$D = \frac{D_u}{D_n}, \quad a = \frac{\beta K}{\rho}, \quad b = \frac{\gamma}{K\beta}.$$

4.2 Numerical solutions

In Figure **??** we plot numerical solution of Equation **??**. No flux boundary conditions are imposed at $x = 0$ and $x = 150$.

```
import numpy as np
from scipy.integrate import odeint
import matplotlib.pyplot as plt

T=100
L=150

a=0.2
b=0.4
D_u=0.10

N_x=100
N_t=100

t=np.linspace(1,T,N_t)
x=np.linspace(0,L,N_x)

u_0=b+(1-b)*0.5*(1+np.tanh(1*0.5*(x-50)))
n_0=(1-b)*0.5*(1+np.tanh(-1*0.5*(x-50)))

u_0=np.concatenate((u_0,n_0))

dx=L/(N_x-1)
dt=T/(N_t-1)

def LVPDErhs(sol,t):
```

```
    N_x=int(np.ceil(len(sol)/2))

    u=sol[0:N_x]
    n=sol[N_x:2*N_x]



    f_u=np.zeros_like(u)
    f_n=np.zeros_like(u)

    for i in range(1,N_x-2):
      f_u[i]=D_u/dx**2*(u[i-1]-2*u[i]+u[i+1])
    i=0
    f_u[i]=D_u/dx**2*(-u[i]+u[i+1])
    i=N_x-1
    f_u[i]=D_u/dx**2*(u[i-1]-u[i])

    for i in range(1,N_x-2):
      f_n[i]=1/dx**2*(n[i-1]-2*n[i]+n[i+1])
    i=0
    f_n[i]=1/dx**2*(-n[i]+n[i+1])
    i=N_x-1
    f_n[i]=1/dx**2*(n[i-1]-n[i])

    reaction_u=u*(1-u-n)
    reaction_n=a*n*(u-b)

    f_u=f_u+reaction_u
    f_n=f_n+reaction_n

    f= np.concatenate((f_u, f_n))
    return f

sol=odeint(LVPDErhs,u_0,t)

u=sol[:,0:N_x]
n=sol[:,N_x:2*N_x]

fig, ax = plt.subplots(2,1)

ax[0].plot(x,u[0,:],'r')
```

```
ax[0].plot(x,u[16,:],'b')
ax[0].plot(x,u[32,:],'m')
ax[0].plot(x,u[48,:],'k')
ax[0].set_xlabel('$x$')
ax[0].set_ylabel('$u$')

ax[1].plot(x, n[0,:],'r--')
ax[1].plot(x, n[16,:],'b--')
ax[1].plot(x, n[32,:],'m--')
ax[1].plot(x, n[48,:],'k--')
ax[1].set_xlabel('$x$')
ax[1].set_ylabel('$n$')

plt.legend(['t'+ str(t[0]),'t='+ str(t[4]),'t='+ str(t[8]),'t='+ str(t[12])])
plt.xlabel('$x$')
plt.grid()
plt.show()
```

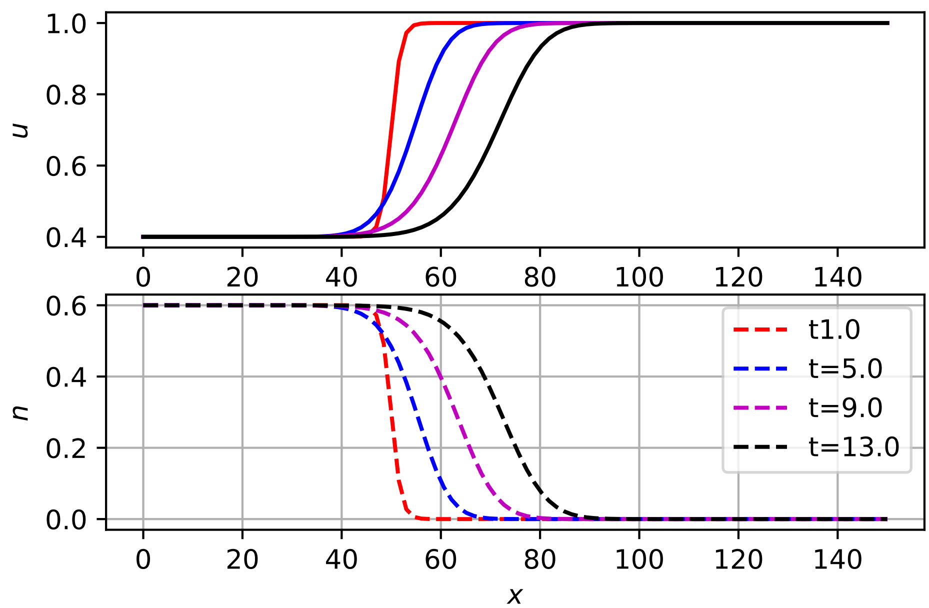

Figure 4.1: Numerical solution of LV model. a=0.2. b=0.4.

4.3 Spatially homogeneous steady states

We firstly consider spatially homogeneous steady states, i.e.

$$f(u,n) = 0, \quad g(u,n) = 0.$$

Thus

$$\begin{aligned} &u(1-u-n) = 0, \quad u = 0, \quad u+n = 1, \\ &an(u-b) = 0, \quad n = 0, \quad u = b. \end{aligned}$$

Thus the steady states are

$$(u_1^*, n_1^*) = (0,0), \quad (u_2^*, n_2^*) = (1,0), \quad (u_3^*, n_3^*) = (b, 1-b),\, 0 \le b < 1.$$

4.4 Stability of steady states to spatially homogeneous perturbations

The Jacobian matrix is

$$J(u_j^*, n_j^*) = \begin{pmatrix} 1-2u-n & -u \\ an & a(u-b) \end{pmatrix}_{(u_j^*, n_j^*)}, \quad j = 1,2,3.$$

For

$$(u_1^*, n_1^*) = (0,0)$$

$$\det(J(0,0) - \lambda I) = -(1-\lambda)(\lambda + ab) = 0$$

and

$$\lambda_1^+ = 1, \quad \lambda_1^- = -ab < 0.$$

Thus $(0,0)$ is a saddle point.

For

$$(u_2^*, n_2^*) = (1,0)$$

$$\det(J(1,0) - \lambda I) = -(1+\lambda)(a(1-b) - \lambda) = 0$$

and

$$\lambda_2^- = -1, \quad \lambda_2^+ = a(1-b) > 0 \ \text{ for } \ 0 \le b < 1.$$

Thus $(1,0)$ is a saddle point.

For $(u_3^*, n_3^*) = (b, 1-b)$

$$\det(J(b, 1-b) - \lambda I) = \lambda^2 + b\lambda + ab(1-b) = 0.$$

If

$$4ab(1-b) \leq b^2 \implies \lambda_3^{\pm} < 0.$$

Hence $(b, 1-b)$ is a stable node.

If

$$4ab(1-b) > b^2 \qquad \implies \Re(\lambda_3 \pm) < 0, \Im(\lambda_3^{\pm}) \neq 0.$$

Hence $(b, 1-b)$ is a stable focus (spiral).

For $b > 0$, $1-b > 0$ spiral oscillations are biologically realistic so long $u > 0$ and $n > 0$.

4.5 Existence of travelling wave profiles connection $(1, 0)$ and $(b, 1-b)$

We make travelling wave *ansatz*

$$\begin{aligned} u(t, x) &= W(x + vt) = W(z), \quad v > 0, \\ n(t, x) &= N(x + vt) = N(z), \quad v > 0, \end{aligned}$$

in Equation **??** and consider the boundary conditions

$$\begin{aligned} u(t,x) &\to 1 \text{ as } x \to -\infty, & W(z) &\to 1 \text{ as } z \to -\infty, \\ u(t,x) &\to b \text{ as } x \to +\infty, & W(z) &\to b \text{ as } z \to +\infty, \\ n(t,x) &\to 0 \text{ as } x \to -\infty, & N(z) &\to 0 \text{ as } z \to -\infty, \\ n(t,x) &\to 1-b \text{ as } x \to +\infty, & N(z) &\to 1-b \text{ as } z \to +\infty. \end{aligned}$$

The system Equation **??** transforms to

$$\begin{aligned} v\frac{dW}{dz} &= D\frac{d^2W}{dz^2} + W(1 - W - N), \\ v\frac{dN}{dz} &= \frac{d^2N}{dz^2} + aN(W - b), \end{aligned}$$

with boundary conditions given by

$$\begin{aligned} W(z) &\to 1 \text{ as } z \to -\infty, \quad W(z) \to b \text{ as } z \to +\infty, \\ N(z) &\to 0 \text{ as } z \to -\infty, \quad N(z) \to 1-b \text{ as } z \to +\infty. \end{aligned} \tag{4.3}$$

Upon making the assumption that the prey moves much more slowly than the predator species, i.e.

$$D = D_u/D_n \ll 1,$$

Equation **??** simplify to

$$\begin{aligned} v\frac{dW}{dz} &= W(1-W-N), \\ v\frac{dN}{dz} &= \frac{d^2N}{dz^2} + aN(W-b). \end{aligned} \tag{4.4}$$

We can rewrite Equation **??** as a system of first order ODEs:

$$\begin{aligned} \frac{dW}{dz} &= \frac{1}{v}W(1-W-N) = F(W,N,P), \\ \frac{dN}{dz} &= P = G(W,N,P), \\ \frac{dP}{dz} &= vP - aN(W-b) = R(W,N,P). \end{aligned} \tag{4.5}$$

The steady states of Equation **??** are

$$\begin{aligned} (W_1^*, N_1^*, P_1^*) &= (0,0,0), \\ (W_2^*, N_2^*, P_2^*) &= (1,0,0), \\ (W_3^*, N_3^*, P_3^*) &= (b, 1-b, 0). \end{aligned}$$

The Jacobian matrix is

$$J(W,N,P) = \begin{pmatrix} \frac{1}{v} - \frac{2W}{v} - \frac{N}{v} & -\frac{W}{v} & 0 \\ 0 & 0 & 1 \\ -aN & a(b-W) & v \end{pmatrix}.$$

At

$$(W_1^*, N_1^*, P_1^*) = (0,0,0)$$

we have

$$\det(J(0,0,0) - \lambda I) = \left(\frac{1}{v} - \lambda\right)(\lambda^2 - \lambda v - ab) = 0$$

and

$$\lambda_1^1 = \frac{1}{v} > 0, \quad \lambda_2^{\pm} = \frac{v \pm \sqrt{v^2 + 4ab}}{2}$$

Thus $(0,0,0)$ is a saddle point with a 2-dim unstable manifold

At $(W_2^*, N_2^*, P_2^*) = (1,0,0)$ we have

$$\det(J(1,0,0) - \lambda I) = \left(-\frac{1}{v} - \lambda\right)(\lambda^2 - \lambda v + a(1-b)) = 0$$

and

$$\lambda_1^1 = -\frac{1}{v} < 0, \quad \lambda_2^{\pm} = \frac{v \pm \sqrt{v^2 - 4a(1-b)}}{2}$$

Thus since, $0 \leq b < 1$ and $4(1-b) > 0$,

$$\begin{array}{ll} \text{If} \quad v^2 \geq 4a(1-b) & (1,0,0) \text{ is a saddle with 2-dim unstable manifold,} \\ \text{If} \quad v^2 < 4a(1-b) & (1,0,0) \text{ is an unstable focus} \end{array}$$

Thus for a travelling wave with $W \geq 0$ and $N \geq 0$ to exist we require

$$v^2 \geq 4a(1-b)$$

and obtain a minimal wave speed

$$v_{\min} = 2\sqrt{a(1-b)} \quad \text{with} \quad 0 \leq b < 1.$$

At $(W_3^*, N_3^*, P_3^*) = (b, 1-b, 0)$ we have

$$\det(J(b,1-b,0) - \lambda I) = \lambda^3 - \lambda^2(v - \frac{b}{v}) - \lambda b - \frac{1}{v}ab(1-b) = p(\lambda) = 0.$$

It can be shown that the extrema of $p(\lambda)$ are independent of the parameter a.

To identify extrema, we compute

$$p'(\lambda) = 3\lambda^2 - 2\lambda\left(v - \frac{b}{v}\right) - b = 0$$

and find that

$$\lambda_{m,M} = \frac{1}{3}\left[\left(v - \frac{b}{v}\right) \pm \sqrt{\left(v - \frac{b}{v}\right)^2 + 3b}\right].$$

If $a = 0$, the eigenvalues are

$$\lambda_3^1 = 0, \quad \lambda_3^{\pm} = \frac{1}{2}\left(v - \frac{b}{v} \pm \sqrt{\left(v - \frac{b}{v}\right)^2 + 4b}\right).$$