

# Lecture slides

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# Lecture 1

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

## Conservation equations

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

## Spatially homogeneous models (MA32009 revision)

## Example problem - bacteria in a dish

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

## A model for cell growth under nutrient depletion

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

## Leading to the logistic growth equation

The last equation can be rewritten as

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

Can also consider other biological processes



## Exercise

Consider a well mixed bio reactor.

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

Cells undergo division with a period of 14 h.

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

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

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

# Model development

## **i** Model checklist

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

## Exercise solution

# Recap

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

## Lecture 2

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

## Exercise

Consider a well mixed bio reactor.

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

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

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

## The SIR model (used in Chapter 7)

Consider the SIR model equations:

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

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

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

What are the variables? What are the parameters?

Identify an expression for the reproduction number,  $R_0$ .

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

## SIR model Calculations

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

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

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

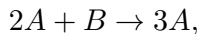


## An activator inhibitor model (used in Chapter 6)

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

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

Consider the reaction schematic



with reaction rate  $k_3$ .

Write down governing ODEs.

## Activator-inhibitor model

Consider the ODEs

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

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

# Recap

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

## Lecture 3 Spatiotemporal models

- ▶ Derive conservation PDEs
- ▶ Consider different models of fluxes

## Spatiotemporal models - derivation

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

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

## Deriving a conservation equation in 1D

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

## A conservation PDE in 1D

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

## Generalising to $R^n$

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



## Fluxes - Fickian diffusion

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

## Fluxes - Nonlinear diffusion

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

Hence

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

## Fluxes - Convection/advection

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

## Fluxes - Taxis

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

Domain of definition of the problem

# Lecture 4

- ▶ Boundary and initial conditions
- ▶ Nondimensionalisation
- ▶ Model formulation

## Boundary conditions

- ▶ Dirichlet
- ▶ Neumann
- ▶ Robin

Initial conditions



## Formulating a model

## Lecture 5

- ▶ Introduce a linear reaction diffusion model
- ▶ Diffusion

## Linear reaction diffusion equation

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

so in 1D Cartesian coordinates

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

## 1D diffusion equation with delta IC

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

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

where  $\delta_0$  is a *Dirac delta distribution* (Dirac measure) satisfying

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

# Numerical solution

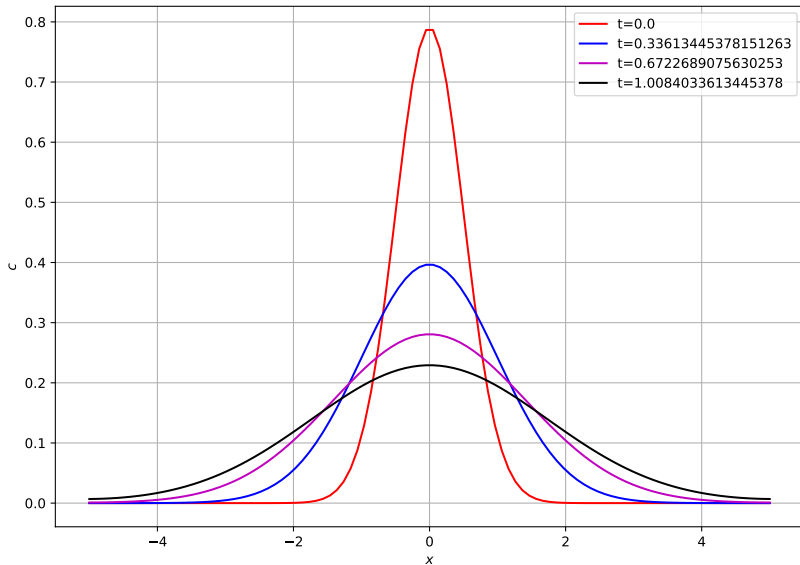


Figure 1: Numerical solution of diffusion equation.

## An exact solution computed using a *similarity* variable

Consider the diffusion Equation 7 with initial condition Equation 8.

Introduce the similarity variable

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

and look for solution of the form

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

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

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

# The 1D diffusion equation for arbitrary initial condition

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

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

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

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



## Diffusive transit time

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

## Diffusion as a description of random walk

Suppose that the probability of a particle hopping distance  $\Delta x$  to the right in time  $\Delta t$  is

$$\lambda_R \Delta t.$$

Similarly, the probability of hopping a distance  $\Delta x$  to the left is

$$\lambda_L \Delta t.$$

# Numerical simulation

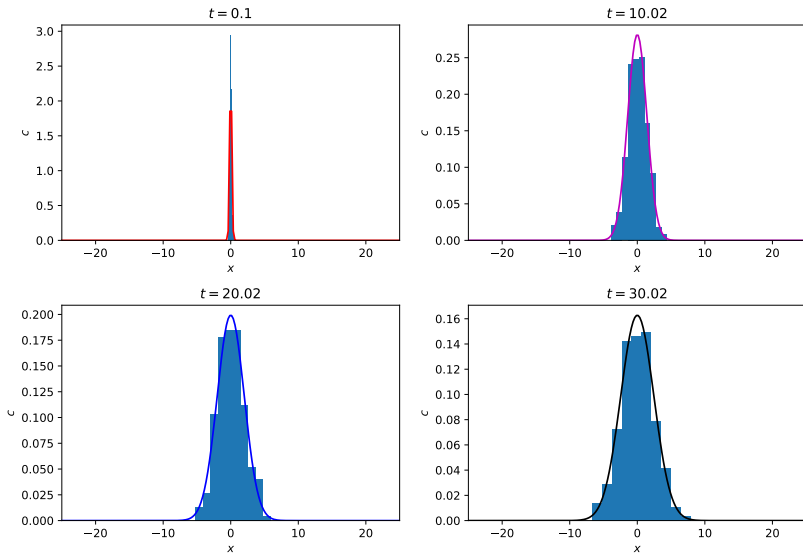


Figure 3: Numerical implementation of random walk

## Derivation

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

A conservation equation for  $c$  is given by

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

## Lecture 6

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

## Recap from last week

A conservation equation for  $c$  is given by

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



## Linear reaction term

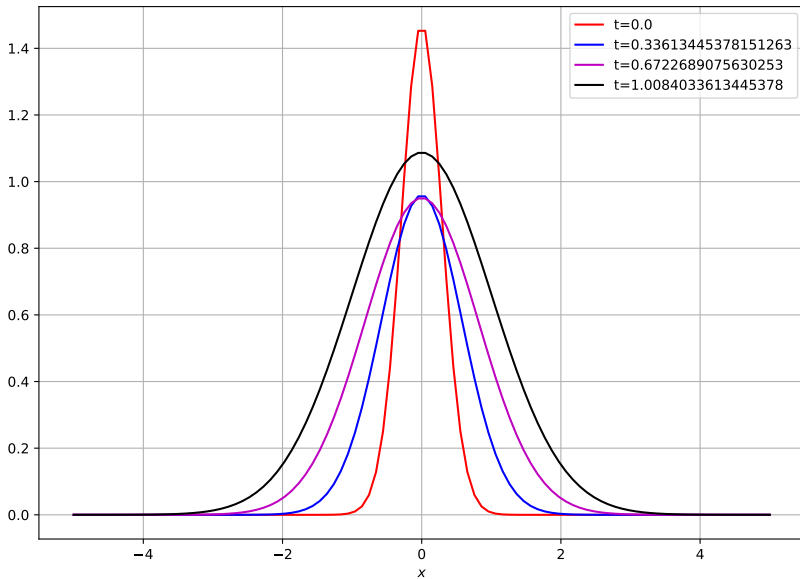
$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} + \rho c, \quad x \in \mathbb{R}, \quad t > 0, \quad (10)$$

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

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



# Numerical solution



## Muskrat invasion dynamics

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

with initial condition

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

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

## Lecture 7

# Travelling waves

## **i** Travelling wave

A travelling wave is a solution of a PDE that has a constant profile (shape) and a constant propagation speed.

## Fisher's equation

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

with initial condition

$$u(x, 0) = u_0(x). \tag{13}$$

## Nondimensional form

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

with initial condition

$$u(x, 0) = u_0(x). \tag{14}$$

## Numerical solution

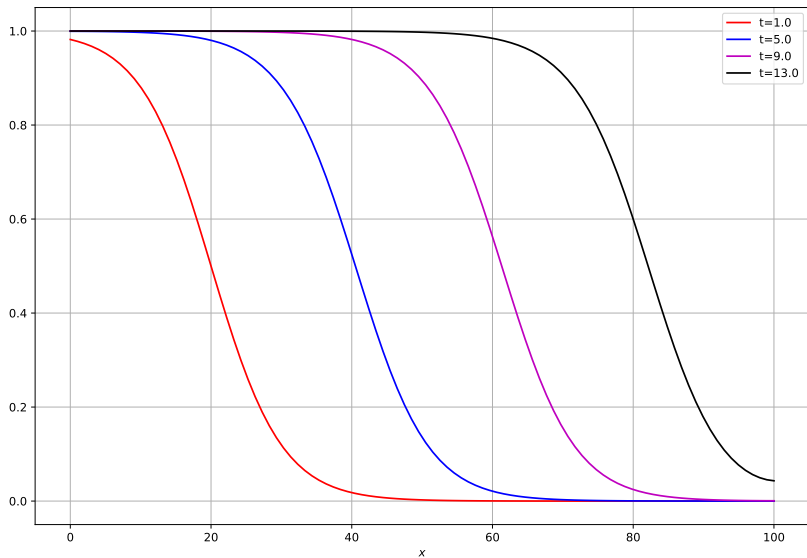


Figure 4: Numerical solution of Fisher's equation.

## Spatially homogeneous solutions



# Travelling wave solutions

In travelling wave coordinates

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

## A pair of first order ODEs

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

$$\frac{dP}{dz} = -vP - W(1 - W) = G(W, P).$$

## Numerical solution

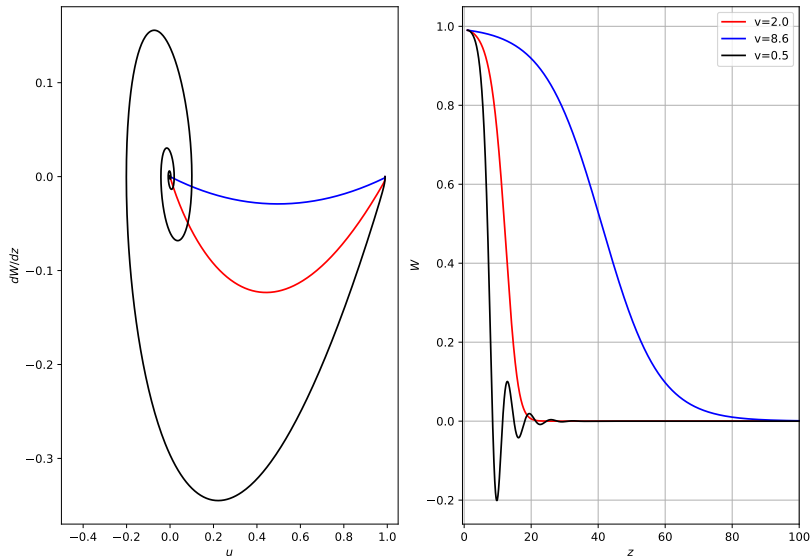


Figure 5: Numerical solution of the travelling wave problem in the phase plane

## Lecture 8 Recap

- ▶ Two steady states (saddle plus stable node)
- ▶ Confined set
- ▶ no oscillations

### **i** PDE

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

### **i** Travelling wave solution

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

## Recap

**i** Pair of first order ODEs

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

Steady state:  $(0,0)$ ,  $(1,0)$

# Linear stability analysis

$(0,0)$  is either a stable node or a stable spiral

$(1,0)$  is a saddle



A heteroclinic trajectory

A minimal wave speed

# Existence of a travelling wave solution

Strategy:

- ▶ identify a confined set in  $\mathfrak{R}^2$
- ▶ show no other steady states in confined set
- ▶ show no oscillatory solutions

Hence: trajectory that leaves  $(1,0)$  via unstable manifold must connect to stable manifold at  $(0,0)$

## A confined set

Consider

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

for some  $\mu < 0$ .

A confined set - ctd

## Lecture 8 Recap

- ▶ Two steady states (saddle + stable node)
- ▶ Confined set
- ▶ No oscillations

Finishing off the confined set

## No oscillations

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

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

has no periodic solutions in this region.



## Choosing $\phi$

For any  $v > 2$ , there exists a travelling wave solution to Fisher's equation.

## Sign of the wave speed

Consider the travelling wave ODE

$$\frac{d^2W}{dz^2} + vW + W(1 - W) = 0$$

## The bistable equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f(u), \quad x \in \mathbb{R}, \quad t > 0, \quad (15)$$

with initial condition

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

Let

$$f(0) = f(a) = f(1) = 0, \quad \text{with } 0 < a < 1.$$

There are therefore three spatially uniform steady states  $u_1 = 0$ ,  $u_2 = a$ ,  $u_3 = 1$ .

$$f'(0) < 0, \quad f'(a) > 0 \quad \text{and} \quad f'(1) < 0$$

$$f = u(u - a)(1 - u),$$

which arises in the study of nerve action potentials along nerve fibres and other problems in *excitable media*

(Gilkey, 1992, ch. 10, §10.1)

## Numerical solution

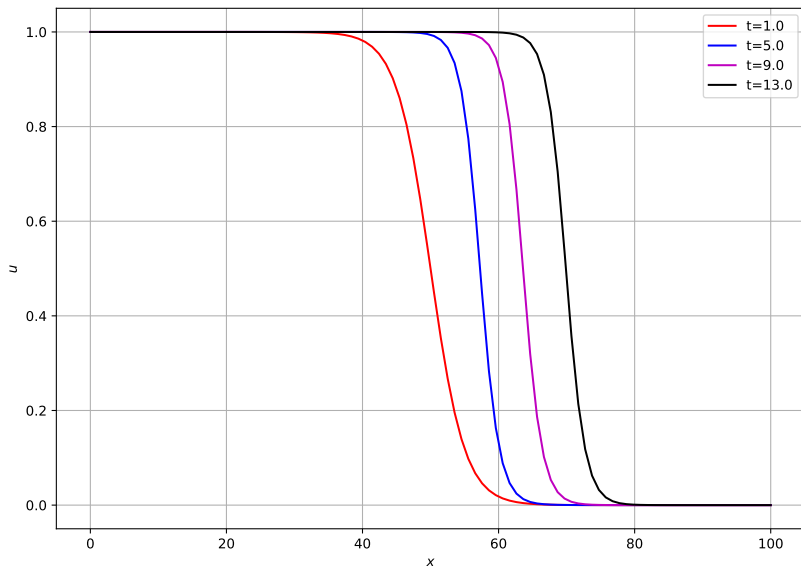


Figure 6: Travelling waves in a numerical solution of bistable PDE.

## Lecture 9

- ▶ Bistable equation

## Travelling wave ansatz

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

In the phase plane

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

# Steady states and their linear stability





The sign of  $v$

## Lecture 10

Recap: travelling wave analysis of bistable equation

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

# Numerical shooting

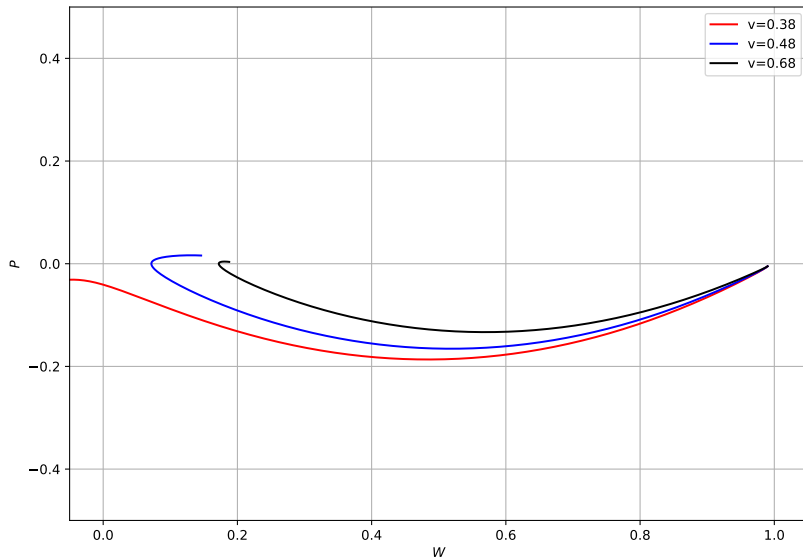


Figure 7: Using a shooting method to investigate travelling wave solutions. Continuity arguments suggest that there exists a travelling

# A shooting method to prove the existence of a traveling wave

## Outline

Trajectories with small  $v$  intersect the  $P$  axis with  $P < 0$

Assume that

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

Trajectories with large  $v$  intersect the  $W$  axis with  $W > 0$

Continuity there exists a trajectory with intermediate  $v$  that passes through the origin

Systems of coupled reaction diffusion equations



## Lotka Volterra with diffusion

$$\begin{aligned}\frac{\partial u}{\partial t} &= \rho u \left(1 - \frac{u}{K}\right) - \alpha u n + D_u \Delta u, \\ \frac{\partial n}{\partial t} &= \beta u n - \gamma n + D_n \Delta n,\end{aligned}\tag{16}$$

## Nondimensional form

$$\begin{aligned}\frac{\partial u}{\partial t} &= u(1 - u - n) + D \frac{\partial^2 u}{\partial x^2} = f(u, n) + D \frac{\partial^2 u}{\partial x^2}, & x \in \mathbb{R}, t > 0, \\ \frac{\partial n}{\partial t} &= a n(u - b) + \frac{\partial^2 n}{\partial x^2} = g(u, n) + \frac{\partial^2 n}{\partial x^2}, & x \in \mathbb{R}, t > 0, \\ & & (17)\end{aligned}$$

## Spatially homogeneous steady states

# Lecture 11

## Recap

$$\begin{aligned}\frac{\partial u}{\partial t} &= u(1 - u - n) + D \frac{\partial^2 u}{\partial x^2} = f(u, n) + D \frac{\partial^2 u}{\partial x^2}, & x \in \mathbb{R}, t > 0, \\ \frac{\partial n}{\partial t} &= a n(u - b) + \frac{\partial^2 n}{\partial x^2} = g(u, n) + \frac{\partial^2 n}{\partial x^2}, & x \in \mathbb{R}, t > 0,\end{aligned}$$

Spatially hom. steady states:

- ▶  $(0, 0)$  - extinction - lin. unstable
- ▶  $(1, 0)$  - no predator, lin unstable
- ▶  $(b, 1 - b)$  - coexistence - lin. stable

Question: do travelling wave solutions exist that connect the spatially homogeneous stable steady state to either of the unstable steady states?

A travelling wave that connects  $(1, 0)$  and  $(b, 1 - b)$

$$u(x, t) = W(x + vt) = W(z), \quad v > 0,$$

$$n(x, t) = N(x + vt) = N(z), \quad v > 0.$$

## The limit of fast diffusing predator

## Three first order ODEs

$$\begin{aligned}\frac{dW}{dz} &= \frac{1}{v}W(1 - W - N) = F(W, N, P), \\ \frac{dN}{dz} &= P = G(W, N, P), \\ \frac{dP}{dz} &= vP - aN(W - b) = R(W, N, P).\end{aligned}\tag{18}$$

# Steady states and their linear stability



# Steady states and their linear stability

## Lecture 12

- ▶ steady states:  $(0, 0, 0)$ ,  $(1, 0, 0)$ ,  $(b, 1 - b, 0)$
- ▶ Heteroclinic trajectory from  $(1, 0, 0)$  to  $(b, 1 - b, 0)$
- ▶  $(1, 0, 0)$  has a 2 dim unstable manifold
- ▶ Eigenvalues at  $(b, 1 - b, 0)$  satisfy

$$\lambda^3 - \lambda^2\left(v - \frac{b}{v}\right) - \lambda b - \frac{1}{v}ab(1 - b) = p(\lambda) = 0.$$

TPs are independent of  $a$

$p(\cdot)$  has a real positive root and two roots with negative real part

## Plotting the cubic

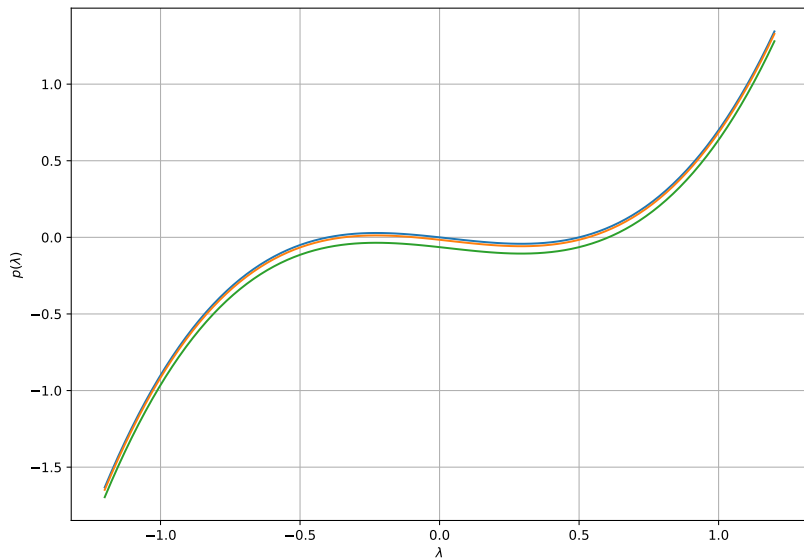


Figure 8: Plot of cubic.

## Aggregation via chemotaxis

- ▶ *Dictyostelium discoideum* (Dicty) is a slime-mold that is widely studied experimentally as a model organism.
- ▶ under nutrient starvation, it exhibits complex collective behaviour
- ▶ individual amoebae that constitute a slime-mold exhibit a range of phenomena also observed in mammalian cells e.g. differentiation, proliferation, migration.



Figure 9: Spiral wave patterns underlying Dictyostelium aggregation.

How do simple rules give rise to complex behaviours?

## A chemotactic model

A 1D spatial domain with no-flux boundary conditions



## Lecture 13

Domain:

$$x \in [0, L], t > 0$$

PDE:

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} - \chi_0 \frac{\partial}{\partial x} \left( n \frac{\partial a}{\partial x} \right),$$

$$\frac{\partial a}{\partial t} = D_a \frac{\partial^2 a}{\partial x^2} + \mu n - \delta a,$$

(19)

Boundary conditions:

$$\frac{\partial a}{\partial x} = \frac{\partial n}{\partial x} = 0, \quad x = 0, L.$$

ICs:

## numerical solution

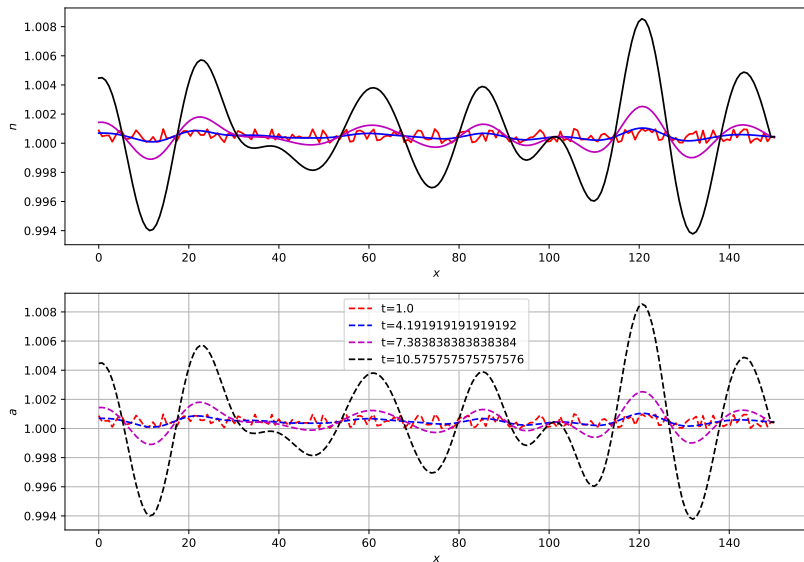


Figure 10: Numerical solution of bacterial chemotaxis model.

## Conservation of cell number

## Spatially homogeneous solutions

## Linearisation about the spatially homogeneous steady state

$$n(x, t) = n^* + \tilde{n}(x, t), \quad a(x, t) = a^* + \tilde{a}(x, t)$$

## Separable solution

$$\tilde{n}(t, x) = u(t)\phi_1(x), \quad \tilde{a}(t, x) = v(t)\phi_2(x)$$

## The elliptic problem

$$\begin{aligned}\frac{d^2\phi}{dx^2} &= -k^2\phi && \text{in } (0, L), \\ \frac{d\phi}{dx} &= 0 && \text{for } x = 0, x = L.\end{aligned}$$

$$\phi_1 = \phi_2 = \phi$$



## Linear system solution

$$u(t) = C_1 e^{\lambda t} \quad \text{and} \quad v(t) = C_2 e^{\lambda t}$$

## Lecture 13 - Recap

Domain:

$$x \in [0, L], t > 0$$

PDE:

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} - \chi_0 \frac{\partial}{\partial x} \left( n \frac{\partial a}{\partial x} \right),$$

$$\frac{\partial a}{\partial t} = D_a \frac{\partial^2 a}{\partial x^2} + \mu n - \delta a,$$

(20)

Boundary conditions:

$$\frac{\partial a}{\partial x} = \frac{\partial n}{\partial x} = 0, \quad x = 0, L.$$

ICs:

# Method

- ▶ Linearise about the steady state
- ▶ Separation of variables  $\tilde{n}(x, t) = u(t)\phi(x)$   $\tilde{a}(x, t) = v(t)\phi(x)$
- ▶ Eigenvalues of the Laplacian operator

$$\frac{d^2\phi}{dx^2} = -k^2\phi, \quad k = \frac{\bar{n}\pi}{L}, \bar{n} \in \mathbb{Z}$$

- ▶ Linear ODEs in  $u(t)$  and  $v(t)$
- ▶ For instability of spatially homogeneous steady state, require  $\Re\{\lambda > 0\}$ .

## Eigenvalue equation

$$\lambda^2 + (D_n k^2 + D_a k^2 + \delta) \lambda + D_n k^2 (D_a k^2 + \delta) - \mu \chi_0 n^* k^2 = 0.$$

Conditions for instability of spatially homogeneous pattern

## Lecture 16 - Diffusion driven instability

$$\begin{aligned}\frac{\partial A}{\partial t} &= F(A, B) + D_A \nabla^2 A, \\ \frac{\partial B}{\partial t} &= G(A, B) + D_B \nabla^2 B,\end{aligned}$$

# Reaction kinetics

Schnackenberg

$$F(A, B) = k_1 - k_2 A + k_3 A^2 B, \quad G(A, B) = k_4 - k_3 A^2 B$$

Gierer Meinhardt:

$$F(A, B) = k_1 - k_2 A + \frac{k_3 A^2}{B}, \quad G(A, B) = k_4 A^2 - k_5 B$$

Thomas:

$$\begin{aligned} F(A, B) &= k_1 - k_2 A - H(A, B), \\ G(A, B) &= k_4 A^2 - k_4 B - H(A, B), \\ H(A, B) &= \frac{k_5 AB}{k_6 + k_7 + k_8 A^2}. \end{aligned}$$

# Nondimensionalisation of Schnakenberg model

Using the scaling

$$u = A \left( \frac{k_3}{k_2} \right)^{1/2}, \quad v = B \left( \frac{k_3}{k_2} \right)^{1/2}, \quad t^* = \frac{D_A t}{L^2}, \quad x^* = \frac{x}{L},$$

$$\begin{aligned} \frac{\partial u}{\partial t} &= \gamma(a - u + u^2 v) + \nabla^2 u = \gamma f(u, v) + \nabla^2 u, \\ \frac{\partial v}{\partial t} &= \gamma(b - u^2 v) + d \nabla^2 v = \gamma g(u, w) + d \nabla^2 v, \end{aligned} \tag{21}$$



## Interpretation of Schnackenberg model: short range activation/long range inhibition

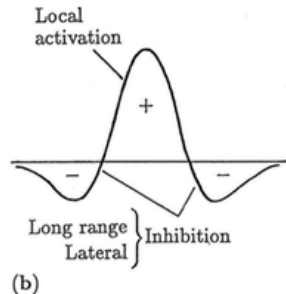
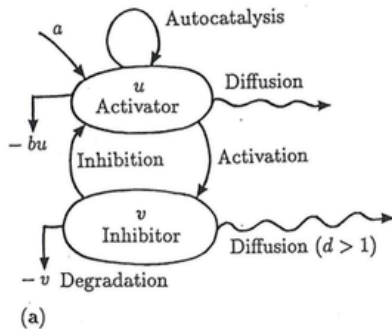


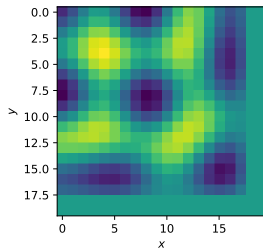
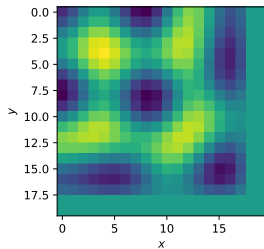
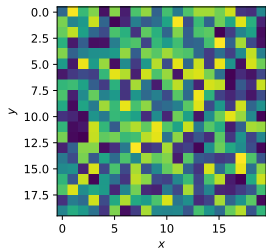
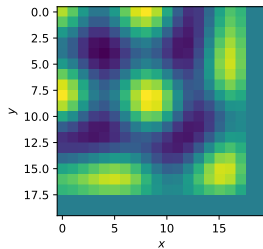
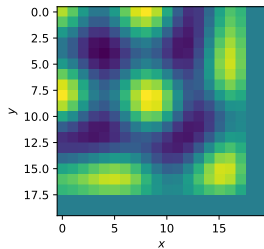
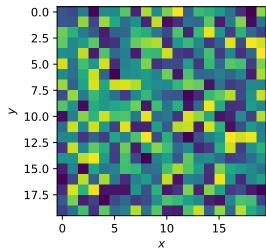
Figure 11

## General form for nondimensionalised RD model

$$\frac{\partial u}{\partial t} = \gamma f(u, v) + \nabla^2 u,$$

$$\frac{\partial v}{\partial t} = \gamma g(u, w) + d \nabla^2 v,$$

# Numerical solution



## Deriving general conditions for diffusion-driven instability

Let  $\Omega \subset R^n$  be a domain with smooth (sufficiently regular) boundary  $\partial\Omega$ , with outward unit normal  $\mathbf{n}$ .

$$\begin{aligned}\frac{\partial u}{\partial t} &= \gamma f(u, v) + \nabla^2 u, & x \in \Omega, \quad t > 0, \\ \frac{\partial v}{\partial t} &= \gamma g(u, v) + d \nabla^2 v, & x \in \Omega, \quad t > 0,\end{aligned}\tag{22}$$

Boundary and initial conditions

$$\begin{aligned}\nabla u \cdot \mathbf{n} &= 0, & \nabla v \cdot \mathbf{n} &= 0, & x \in \partial\Omega, \quad t > 0, \\ u(x, 0) &= u_0(x), & v(x, 0) &= v_0(x), & x \in \Omega.\end{aligned}\tag{23}$$

## Conditions for diffusion driven instability

$$f_u + g_v < 0,$$

$$f_u g_v - f_v g_u > 0,$$

$$df_u + g_v > 0,$$

$$(df_u + g_v)^2 - 4d(f_u g_v - f_v g_u)^2 < 0,$$

## A spatially homogeneous steady-state

A *spatially homogeneous steady-state* of Equation 22 and Equation 23 satisfies

$$f(u_0, v_0) = g(u_0, v_0) = 0.$$

For linear stability

$$\begin{aligned} f_u + g_v &< 0, \\ f_u g_v - f_v g_u &> 0 \end{aligned}$$

Here

$$f_u = \frac{\partial f}{\partial u_{(u_0, v_0)}}$$

etc.

## Spatially dependent perturbations

$$u(x, t) = u_0 + \tilde{u}(x, t), \quad v(x, t) = v_0 + \tilde{v}(x, t), \quad \|\tilde{u}(x, t)\| \ll 1, \quad \|\tilde{v}(x, t)\| \ll 1$$

## Separation of variables

$$V(x, t) = \begin{pmatrix} \bar{u}(t)\varphi_1(x) \\ \bar{v}(t)\varphi_2(x) \end{pmatrix},$$



A set of basis functions

Returning to the vectorised form of equations

A modified Jacobian for spatially heterogeneous perturbations

## Lecture 18 Recap

For linear instability of spatially homogeneous steady state:

$$\det(\tilde{J}) = h(k^2) = dk^4 - \gamma(df_u + g_v)k^2 + \gamma^2 \det(J) < 0.$$

$$df_u + g_v > 0.$$

$$\frac{(df_u + g_v)^2}{4d} > |J|.$$

## Instability for a limited range of wavenumbers

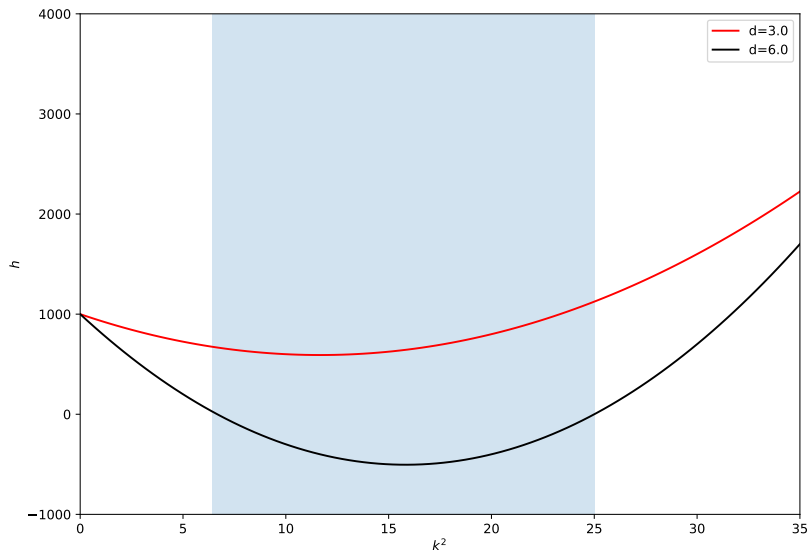


Figure 12: A plot of  $h(k^2)$  plotted against  $k^2$ . Shaded region denotes unstable wave numbers in case of targets  $d$

## Summary - DDI conditions

$$f_u + g_v < 0,$$

$$f_u g_v - f_v g_u > 0,$$

$$df_u + g_v > 0,$$

$$(df_u + g_v)^2 - 4d(f_u g_v - f_v g_u)^2 < 0,$$



# The SIR model

## Assumptions

- ▶ Total population is constant: the duration of the epidemic is short compared to the lifetime of its hosts, so we can neglect birth and disease-unrelated death
- ▶ Consider a disease which, after recovery, confers immunity (and/or death if lethal)
- ▶ Population is well mixed (spatially homogenous)

## SIR model - variables

- ▶  $S$  – susceptibles - can be infected
- ▶  $I$  – infectives - have the disease and can transmit to susceptibles
- ▶  $R$  – recovered (removed) - have had the disease and are no longer infective.

Progress through the disease

$$S \longrightarrow I \longrightarrow R$$

## SIR model - ODEs

$$\begin{aligned}\frac{dS}{dt} &= -rSI, \\ \frac{dI}{dt} &= rSI - aI \\ \frac{dR}{dt} &= aI\end{aligned}\tag{24}$$

Epidemic:

$$rS_0 > a \implies R_0 := \frac{rS_0}{a} > 1$$

## Spatio-temporal model

$$\frac{\partial S}{\partial t} = -rSI + D_S \frac{\partial^2 S}{\partial x^2}, \quad x \in \mathbb{R}, t > 0,$$

$$\frac{\partial I}{\partial t} = rSI - aI + D_I \frac{\partial^2 I}{\partial x^2}, \quad x \in \mathbb{R}, t > 0,$$

$$\frac{\partial R}{\partial t} = aI + D_R \frac{\partial^2 R}{\partial x^2}, \quad x \in \mathbb{R}, t > 0$$

$$S(0, x) = S_0(x), \quad I(0, x) = I_0(x), \quad R(0, x) = R_0(x), \quad x \in \mathbb{R},$$

(25)

# Nondimensionalise

Defining

$$i = \frac{I}{\bar{S}_0}, s = \frac{S}{\bar{S}_0}, \quad x^* = \left( \frac{r\bar{S}_0}{D_I} \right)^{1/2} x, \tau = r\bar{S}_0 t$$

we obtain ( after dropping '\*' )

$$\frac{\partial s}{\partial t} = -si + d \frac{\partial^2 s}{\partial x^2}, \quad x \in \mathbb{R}, t > 0,$$

$$\frac{\partial i}{\partial \tau} = si - \mu i + \frac{\partial^2 i}{\partial x^2}, \quad x \in \mathbb{R}, t > 0,$$

$$s(x, 0) = \frac{S_0(x)}{\bar{S}_0}, \quad i(x, 0) = \frac{I_0(x)}{\bar{S}_0}, \quad x \in \mathbb{R},$$

where  $\bar{S}_0$  is a representative population density and  $\mu = a/r\bar{S}_0$ .

# Aim

- ▶ investigate the spatial spread of an epidemic wave of infectives into a uniform susceptibles population  $S_0(x) = \bar{S}_0$ .
- ▶ determine conditions for existence of an epidemic wave and propagation speed.

## Boundary conditions

$$\begin{array}{llll} \bar{s}(z) \rightarrow 1 & z \rightarrow +\infty, & \bar{i}(z) \rightarrow 0 & z \rightarrow +\infty, \\ \bar{s}(z) \rightarrow \sigma & z \rightarrow -\infty, & \bar{i}(z) \rightarrow 0 & z \rightarrow -\infty, \\ \bar{s}'(z) \rightarrow 0 & z \rightarrow \pm\infty, & \bar{i}'(z) \rightarrow 0 & z \rightarrow \pm\infty, \end{array} \quad (26)$$

where  $0 \leq \sigma < 1$ .

## Travelling wave analysis

$$s(x, t) = \bar{s}(z), \quad i(x, t) = \bar{i}(z), \quad z = x - vt, \quad v > 0$$

$$\begin{aligned}\bar{s}'' + v\bar{s}' - \bar{i}\bar{s} &= 0, \\ \bar{i}'' + v\bar{i}' + \bar{i}\bar{s} - \mu\bar{i} &= 0.\end{aligned}\tag{27}$$



## Steady states of the travelling wave problem

$$(s^*, i^*) = (1, 0), \quad (s^*, i^*) = (\sigma, 0)$$