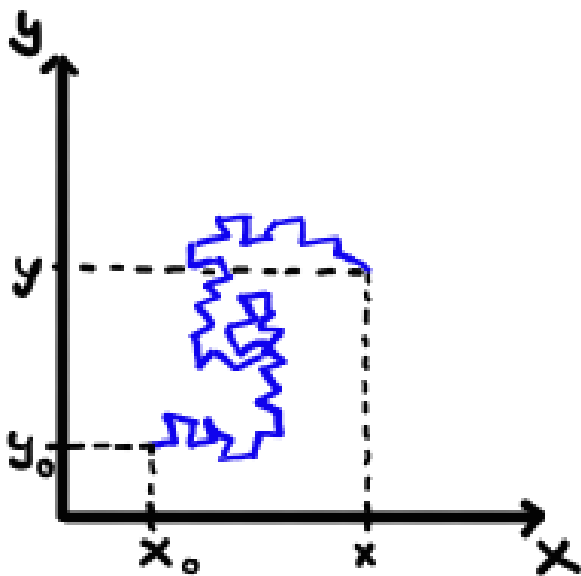


6 Reaction-diffusion equations & travelling waves (Murray, Ch. 11, 13)

6.1 Diffusion

In lecture 5 we introduced one-dimensional random walks and derived a diffusion equation that determines the probability to find a random walker at position x at time t . The phenomenology of diffusion is similar in higher dimensions. Consider for example Brownian motion, i.e. the random motion of a particle induced by collisions with many smaller molecules:



Similar to the one-dimensional case, the mean square displacement for a particle initially localized at (x_0, y_0) grows linearly with time:

$$\text{var}(x - x_0) = 2Dt, \quad \text{var}(y - y_0) = 2Dt,$$

where D is the diffusion coefficient. Individual particles are unlikely to be found at their initial position after long times.

In general diffusion denotes an ‘irreversible’ process by which matter, particle groups, populations etc. spread out within a given space according to ‘random motion’ of individual particles. Here ‘irreversible’ means that the probability to go back to the initial configuration goes to zero as the number of particles goes to infinity. The ‘random motion’ can either be uncorrelated at different time steps, or there can

be some correlations that depend on which underlying mechanisms drives the particles. Three examples of underlying mechanisms important for biological applications are: molecular motion (molecular diffusion), turbulent flow (turbulent diffusion), and self-driven motion (motility) of biological species (population diffusion). As discussed below, the magnitude and spatial dependence of the diffusion coefficients may vary significantly depending on the underlying mechanism.

Example Molecular diffusion of proteins (diffusion coefficient $D \sim 10^{-11}\text{m}^2/\text{s}$) in a cell in the body (length scale $L \sim 10\mu\text{m}$). Time scale for diffusion to homogenise spatial variations of the protein: $T \sim L^2/D \sim 10\text{s}$.

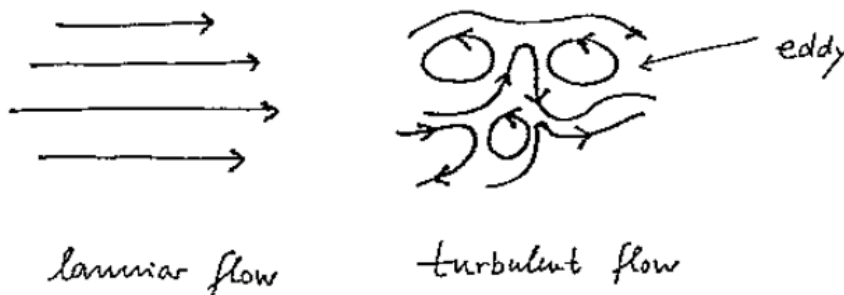
Example Sugar at the bottom of a cup of coffee may spread throughout the cup due to molecular diffusion. The diffusion coefficient for sugar dissolved in coffee is $D \sim 10^{-9}\text{m}^2/\text{s}$. The time T for sugar to get uniformly mixed due to diffusion in a cup of height $L = 5\text{cm}$ is $T \sim L^2/D \sim 30\text{days}$.

6.1.1 Turbulent diffusion (Okubo 2.4)

As seen by the second example above, molecular diffusion is often extremely slow at macroscopic scales. Diffusion due to turbulence is more efficient at these scales. The position of a small particle in a fluid flow evolves as $\dot{\mathbf{x}} = \mathbf{u}(\mathbf{x}, t)$

Laminar flow: low flow velocity \mathbf{u} , streamlines parallel

Turbulent flows: high flow velocity \mathbf{u} , irregular streamlines, chaotic



The accelerations of a particle in a (chaotic) turbulent flow can be viewed as random. The particle is governed by large-scale turbulent

diffusion (as opposed to the molecular-driven diffusion in Brownian motion). Some characteristic features of turbulent diffusion are:

1. Typical time-and length scales in turbulent diffusion are macroscopic (Brownian motion has microscopic length scale).
2. Turbulent flows consist of eddies with sizes that may vary over many orders of magnitude. Which eddies that contribute to the diffusion process varies with length scale ℓ , larger and larger eddies contribute as ℓ is increased. The effective diffusion coefficient $D_{\text{eff.}}$ grows with length scale ℓ as $D_{\text{eff.}} \sim \ell^{4/3}$ according to experiments and theory (Richardson 1926). Turbulent diffusion becomes very efficient at the largest scales (dispersion of particles in the ocean, rain clouds, etc.)
3. Can in general not be modeled by simple random-walk models (need more general correlated random walks)

In conclusion: **Turbulence is very good at mixing (tracer) particles.**

6.1.2 Population diffusion (M11.3,11.4)

In population diffusion the particles (animals) are motile. The diffusion coefficient often depends on the population density. One example is models of migration of humans or animals (demic diffusion) from overcrowded areas into empty areas.

Population diffusion is often directed by chemicals (pheromones) that allow individuals to locate food and other individuals. This is particularly important for small animals that have limited sensing abilities. One example is the diffusion due to ‘run and tumble’ motion of bacteria (run and tumble is essentially a random walk, with alternating steps (run) and reorientations (tumble)). In the presence of a (diffusing) chemical, the run and tumble process may become directed and the bacteria climb the concentration gradient of the diffusing chemical (chemotaxis), leading to a concentration of bacteria close to the source of the chemical.

6.1.3 Importance of diffusion for biological systems

The mechanisms for diffusion discussed above are important in many biological applications. Some examples

- **Motility** All three mechanisms are important to describe the motility and spatial spread of small organisms as well as larger animals (for the latter molecular diffusion is not so important).
- **Reproduction** Spreading of pollen and spores using wind, water, or pollinators relies on all three diffusion mechanisms.
- **Chemical reactions** Molecular diffusion is often the mechanism in which large molecules (proteins and enzymes) are brought into contact with other reactants. Stirring (turbulent diffusion) may increase the reaction rate significantly.
- **Chemical communication** Pheromones from insects and other animals spread through diffusion.
- **Patchiness and pattern formation** can be driven by diffusion processes

This course focuses on population motility and on pattern formation.

6.2 Reaction-diffusion equations (M11.2)

Fick's law (from Lecture 5): diffusion occurs from high concentration to low concentration as to smoothen out concentration gradients. Matter flux (per unit area and unit time)

$$j = -D \frac{\partial n}{\partial x}.$$

Using conservation of mass in a small length segment (continuity equation) we found that Fick's law is equivalent to the one-dimensional diffusion equation.

Now consider a more general situation in three dimensions. Let S be a surface enclosing a volume V :



Apply the **continuity equation (conservation equation)**:

‘Change of concentration in volume V ’

= ‘Outflux of particles through boundary’ + ‘Particle production in volume’

$$\frac{\partial}{\partial t} \int_V d^3\mathbf{x} n(\mathbf{x}, t) = - \int_S \underbrace{d\mathbf{S} \cdot \mathbf{j}(\mathbf{x}, t)}_{\text{flux of particles through } dS} + \int_V d^3\mathbf{x} \underbrace{f(\mathbf{x}, t)}_{\text{source}}$$

Apply divergence theorem

$$\int_S d\mathbf{S} \cdot \mathbf{j}(\mathbf{x}, t) = \int_V d^3\mathbf{x} \nabla \cdot \mathbf{j}(\mathbf{x}, t)$$

to get

$$0 = \int_V d^3\mathbf{x} \left[\frac{\partial}{\partial t} n(\mathbf{x}, t) + \nabla \cdot \mathbf{j}(\mathbf{x}, t) - f(\mathbf{x}, t) \right].$$

This is true for any volume \Rightarrow integrand must vanish at all positions

$$0 = \frac{\partial}{\partial t} n(\mathbf{x}, t) + \nabla \cdot \mathbf{j}(\mathbf{x}, t) - f(\mathbf{x}, t). \quad \text{☑} \quad (1)$$

This is the **differential form of the continuity equation**. It has many applications: n could denote mass, energy, electric charge, etc, and the forms of \mathbf{j} and f are determined by the mechanisms for local flux and production of n . Here, we let n denote a concentration of e.g. a chemical or a population, and we let the local flux \mathbf{j} be governed by diffusion (Fick’s law)

$$\mathbf{j}(\mathbf{x}, t) = -D \nabla n(\mathbf{x}, t).$$

We have

$$\frac{\partial}{\partial t}n(\mathbf{x}, t) = \underbrace{f(\mathbf{x}, t)}_{\text{reaction}} + \underbrace{\nabla \cdot [D \nabla n(\mathbf{x}, t)]}_{\text{diffusion}}. \quad (2)$$

Commonly we let $D = \text{const.}$, but in general D can be **anisotropic (a matrix)** and depend on position (carefully taking into account which of the differential operators ∇ act on D).

Eq. (2) is an example of a **reaction-diffusion equation**: the reaction term describes how concentration n is transformed due to the source f , while the diffusion term describes spatial diffusion of n . The source $f(\mathbf{x}, t)$ is often a functional of concentration n and only implicitly depends on the coordinates \mathbf{x} and t through $n(\mathbf{x}, t)$.

6.2.1 Example: Population growth models

Let the source term $f(\mathbf{x}, t)$ represent birth-and-death processes and $n(\mathbf{x}, t)$ the population density. Assume constant D and logistic growth

$$f(\mathbf{x}, t) = rn \left(1 - \frac{n}{K} \right)$$

with linear growth rate r and carrying capacity K . Use Eq. (2) to get

$$\frac{\partial}{\partial t}n(\mathbf{x}, t) = rn(\mathbf{x}, t) \left(1 - \frac{n(\mathbf{x}, t)}{K} \right) + D \nabla^2 n(\mathbf{x}, t). \quad (3)$$

This is **Fisher's equation**, proposed by Fisher (1937) as a model for the spatial spread of an advantageous gene in a population. It is a natural generalisation of the logistic growth model to include spatial migration via diffusion.

6.2.2 Reaction-diffusion equations in Biological contexts

Reaction-diffusion equations are used to model population migration, infection outbreaks, wound healing, chemical reactions, etc. They also form prototype models for pattern formation. **They are believed to**

be essential for processes in which organisms develop their shape, and for patterns of animal coats and skin pigmentation.

Typical solutions of reaction-diffusion equations are: travelling waves, wave-like phenomena, self-organized patterns like stripes, spirals, etc.

6.2.3 More general reaction-diffusion equation for several interacting species or chemicals

Let $n_\alpha(\mathbf{x}, t)$ with $\alpha = 1, 2, \dots, m$ represent m different species. The reaction-diffusion equation Eq. (2) generalises to

$$\frac{\partial n_\alpha}{\partial t} = f_\alpha + \nabla \cdot \left[\sum_{\beta=1}^m D_{\alpha\beta} \nabla n_\beta \right]$$

The diffusion matrix $D_{\alpha\beta}$ is usually diagonal and interactions between species occur through f_α (each species has its own diffusivity $D_{\alpha\alpha}$).

6.2.4 Advection-diffusion equations

Advection denotes a deterministic transport of a substance with velocity $\mathbf{v}(\mathbf{x}, t)$, for example due to a turbulent fluid flow. The flux

$$\mathbf{j}(\mathbf{x}, t) = \underbrace{\mathbf{v}(\mathbf{x}, t)n(\mathbf{x}, t)}_{\text{Instantaneous flux generated by } \mathbf{v} \text{ (advection)}} - \underbrace{D\nabla n(\mathbf{x}, t)}_{\text{Contribution from diffusion (Fick's law)}}$$

inserted into the continuity equation (1) [neglect source, $f = 0$] gives

$$\frac{\partial}{\partial t}n(\mathbf{x}, t) = -\nabla \cdot \mathbf{j}(\mathbf{x}, t) = \nabla \cdot [-\mathbf{v}(\mathbf{x}, t)n(\mathbf{x}, t) + D\nabla n(\mathbf{x}, t)].$$

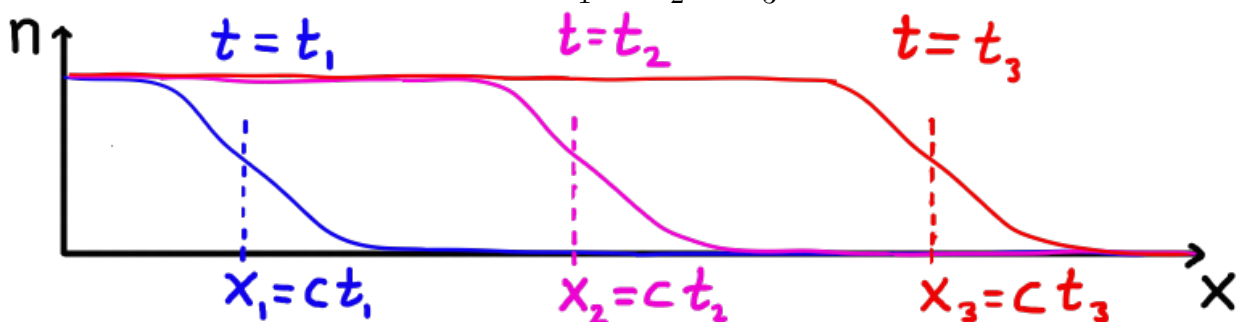
If $\mathbf{v}(\mathbf{x}, t) = \text{const.}$ this is the advection-diffusion equation of the one-dimensional random walk in Lecture 5. More generally when $\mathbf{f} \neq 0$, we have a combination: Reaction-Advection-Diffusion equation.

6.3 Travelling waves (M13.1,13.2,13.5)

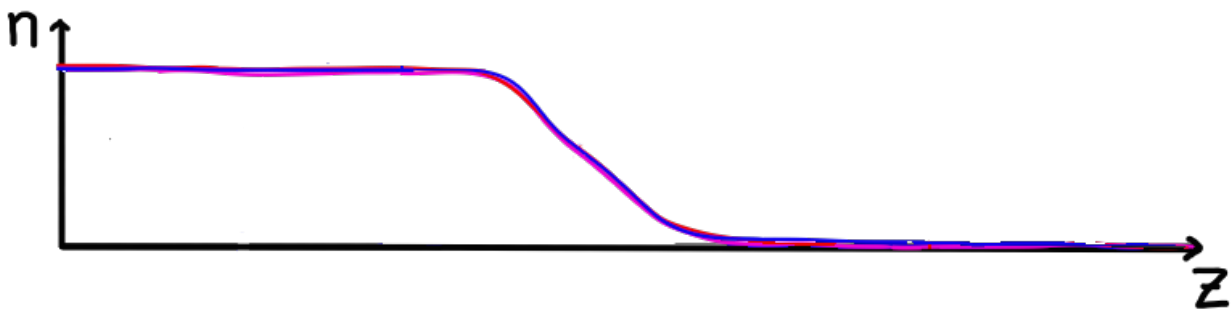
The reaction-diffusion equation in one dimension is

$$\frac{\partial}{\partial t}n(x, t) = f(x, t) + D \frac{\partial^2}{\partial x^2}n(x, t). \quad (4)$$

Assume $f = f(n(x, t))$, i.e. no explicit space-or time-dependence. Typical solutions (depending on f and boundary conditions): waves with continuously varying shape and speed of the wave front. Eq. (4) also allows for travelling-wave solutions: solutions which travel with constant shape and speed (and much faster than diffusion). Illustration for three successive times $t_1 < t_2 < t_3$:



Position of constant n moves with constant speed c . Change coordinates from (x, t) to moving coordinate (z, t) with wave variable $z = x - ct$. The concentration $n(z, t)$ is a travelling wave if it only depends on z (not explicitly on t). For the illustration above all curves collapse:



Depending on the initial condition, the solution may have an initial transient before reaching the travelling wave form. Often travelling waves are stable structures: for many initial conditions the travelling-wave solution is approached at large times.

Now search for travelling wave solutions to Eq. (4) by the ansatz

$$n(x, t) = u(x - ct) = u(z).$$

This coordinate change reduces the number of variables from 2 (x and t) to 1 (z). We have

$$\begin{aligned}\frac{\partial n}{\partial t} &= -c \frac{du}{dz} \\ \frac{\partial n}{\partial x} &= \frac{du}{dz}\end{aligned}$$

and Eq. (4) becomes

$$-c \frac{d}{dz} u(z) = f(u(z)) + D \frac{d^2}{dz^2} u(z), \quad (5)$$

i.e. an ordinary differential equation in z .

Boundary conditions For given boundary+initial conditions Eq. (4) has a unique solution. In contrast, for given boundary conditions Eq. (5) may have different solutions for different values of c .

To find allowed boundary conditions, integrate Eq. (5) over z

$$0 = \left[cu(z) + D \frac{d}{dz} u(z) \right]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} dz f[u(z)].$$

Physical solutions have finite values of $u(z)$ and $u'(z)$ for all z . Therefore the integral must take a finite value. One condition for the integral to be finite is $f[u(z)] \rightarrow 0$ as $z \rightarrow \pm\infty$. Thus, for large $|z|$, $u(z)$ approaches fixed-points $f(u^*) = 0$ of the dynamical system obtained by letting $D = 0$ (homogeneous reaction) in Eq. (5).

6.3.1 Phase-plane analysis

Introduce help variable $v = \frac{du}{dz}$ to rewrite Eq. (5) as first-order system

$$\begin{aligned}\frac{du}{dz} &= v \\ \frac{dv}{dz} &= \frac{-cv - f(u)}{D}\end{aligned}$$

This is a flow with ‘time variable’ z and steady states at $v^* = 0$ and $f(u^*) = 0$. NB: If $c > 0$ then $z = x - ct$ may be of opposite sign compared to $t \Rightarrow$ steady states $f(u^*) = 0$ may show opposite stability compared to homogeneous steady states of Eq. (5) with $D = 0$. Classify the fixed point by evaluation of the Jacobian

$$\mathbb{J} = \begin{pmatrix} 0 & 1 \\ -f'(u^*)/D & -c/D \end{pmatrix}.$$

Eigenvalue equation

$$0 = \det(\mathbb{J} - \lambda \mathbb{I}) = \lambda(\lambda + c/D) + f'(u^*)/D$$

$$\Rightarrow \lambda_{\pm} = \frac{1}{2D} \left(-c \pm \sqrt{c^2 - 4Df'(u^*)} \right)$$

Depending on c , D and $f'(u^*)$ the fixed point can be of any type. Typically: Travelling waves are solutions that connects two steady states (heteroclinic orbit), joining an unstable manifold of the steady state where the wave originates ($z \rightarrow -\infty$) to the stable manifold of the steady state where the wave stops ($z \rightarrow \infty$).

6.3.2 Example: No reaction term

When $f = 0$ (the diffusion equation) no physically meaningful travelling wave exists to Eq. (5)

$$-c \frac{du}{dz} = D \frac{d^2u}{dz^2}$$

$$\Rightarrow u(z) = A + Be^{-cz/D}$$

For the solution to be bounded as $z \rightarrow -\infty$ we must have $B = 0$. The remaining part of solution $n = A = \text{const.}$ is not a wave.

6.3.3 Example: Fisher’s equation (13.2)

$$\frac{\partial n}{\partial t} = \underbrace{rn \left(1 - \frac{n}{K} \right)}_{\text{logistic growth}} + \underbrace{D \frac{\partial^2 n}{\partial x^2}}_{\text{diffusion}}.$$

Change to dimensionless variables (units: $[r] = [t]^{-1}$, $[D] = [x]^2[t]^{-1}$, and $[K] = [n]$)

$$n = Kn', \quad t = \frac{t'}{r}, \quad x = x' \sqrt{\frac{D}{r}} \quad (6)$$

and for convenience drop the primes in what follows, to get

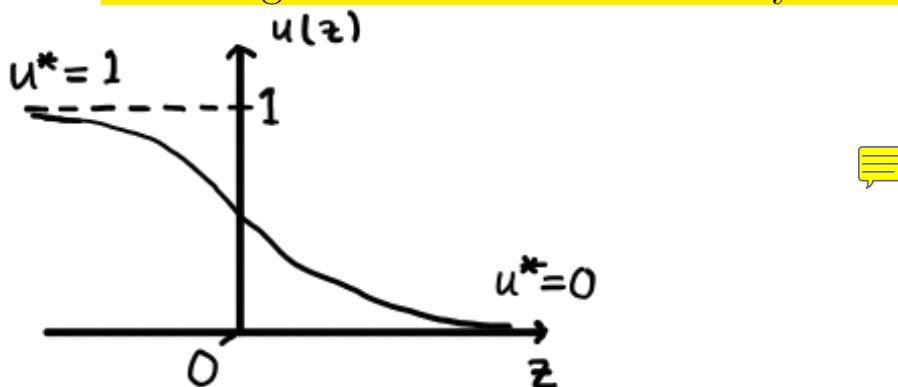
$$\frac{\partial n}{\partial t} = n(1 - n) + \frac{\partial^2 n}{\partial x^2}.$$

If n is independent of x (homogenous solution) this is a dynamical system with two steady states:

$$n^* = 0 \text{ (unstable)}$$

$$n^* = 1 \text{ (stable)}.$$

Idea: Travelling wave connects these steady states:



Search for travelling waves connecting the steady states at large $|z|$ by the ansatz $z = x - ct$ (assume $c \geq 0$):

$$-c \frac{d}{dz} u(z) = u(z) (1 - u(z)) + \frac{d^2}{dz^2} u(z)$$

with boundary conditions

$$\lim_{z \rightarrow -\infty} u(z) = 1$$

$$\lim_{z \rightarrow \infty} u(z) = 0.$$

Introduce help variable $v = \frac{du}{dz}$ to get first order system

$$\begin{aligned}\frac{du}{dz} &= v \\ \frac{dv}{dz} &= -cv - u(1-u) .\end{aligned}$$

This ‘flow’ has two steady states

$$(u^*, v^*) = (0, 0)$$

$$(u^*, v^*) = (1, 0)$$

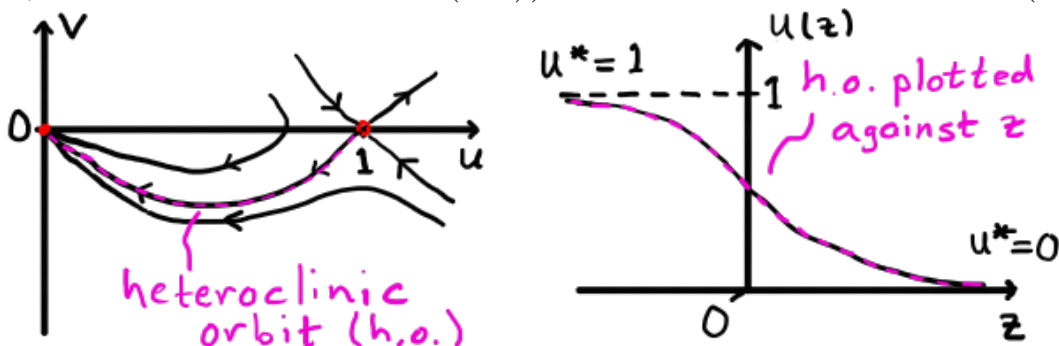
Linearisation

$$\mathbb{J} = \begin{pmatrix} 0 & 1 \\ 2u - 1 & -c \end{pmatrix} .$$

Eigenvalue equation

$$\begin{aligned}0 &= \det(\mathbb{J} - \lambda \mathbb{I}) = \lambda(\lambda + c) - (2u - 1) \\ \Rightarrow \lambda_{\pm} &= \frac{1}{2} \left(-c \pm \sqrt{c^2 + 8u - 4} \right) \\ (u^*, v^*) = (0, 0) : &\begin{cases} \text{stable node} & \text{if } c > 2 \\ \text{stable spiral} & \text{if } c < 2 \end{cases} \\ (u^*, v^*) = (1, 0) : &\text{saddle point} .\end{aligned}$$

Solutions with $c < 2$ are unphysical (u becomes negative when dynamics spiral around $(0,0)$). Phase picture for $c > 2$ (left panel):



The heteroclinic orbit connects the two steady states $u^* = 1$ and $u^* = 0$. The corresponding trajectory is plotted against ‘time’ z in



the right panel starting at $u^* = 1$ as $z \rightarrow -\infty$, ending up at $u^* = 0$ as $z \rightarrow +\infty$, all the way with a negative slope $du/dz = v < 0$. In conclusion, a travelling wave solution exists (the heteroclinic orbit). This is the only physical solution of the system (all other trajectories approach infinity as $z \rightarrow -\infty$ or $z \rightarrow +\infty$).

The travelling-wave solution describes population spread from small values of x to larger values of x in a one-dimensional domain that is initially empty. Changing the sign of c the heteroclinic orbit goes from $u^* = 0$ to $u^* = 1$ in the figure above ($z \rightarrow -z$). This describes a population spread of an initial population at large x that populates an initially empty region at smaller x .

As a final remark, having a non-zero wave speed c always gives a more efficient spread than pure diffusion for large times:

Dispersion mechanism	Diffusion	Travelling wave
Displacement L in time t	$L \sim \sqrt{2Dt}$	$L \sim ct$



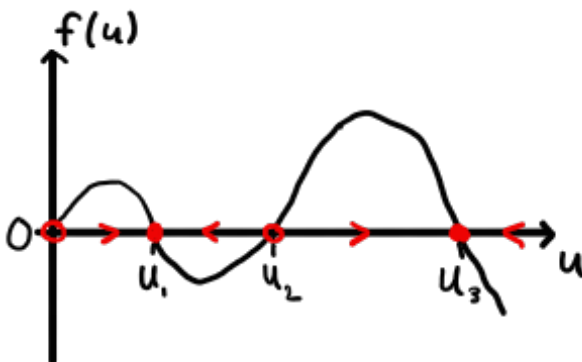
6.3.4 Example: Spruce-budworm model (M13.5)

Consider a reaction-diffusion equation with

$$f(u) = \underbrace{ru(1 - u/q)}_{\text{Logistic growth}} - \underbrace{\frac{u^2}{1 + u^2}}_{\text{Predation}} \quad .$$



Can have more than two fixed points (depending on the parameters):



Two stable steady states: u_1 small population, u_3 outbreak. How does outbreak propagate when spatial dispersion is included?

In the phase plane ($v = du/dz$) corresponding to Eq. (5):

$$\begin{aligned}\frac{du}{dz} &= v \\ \frac{dv}{dz} &= -cv - f(u).\end{aligned}$$

There are four steady states: (assume $c > 0$)

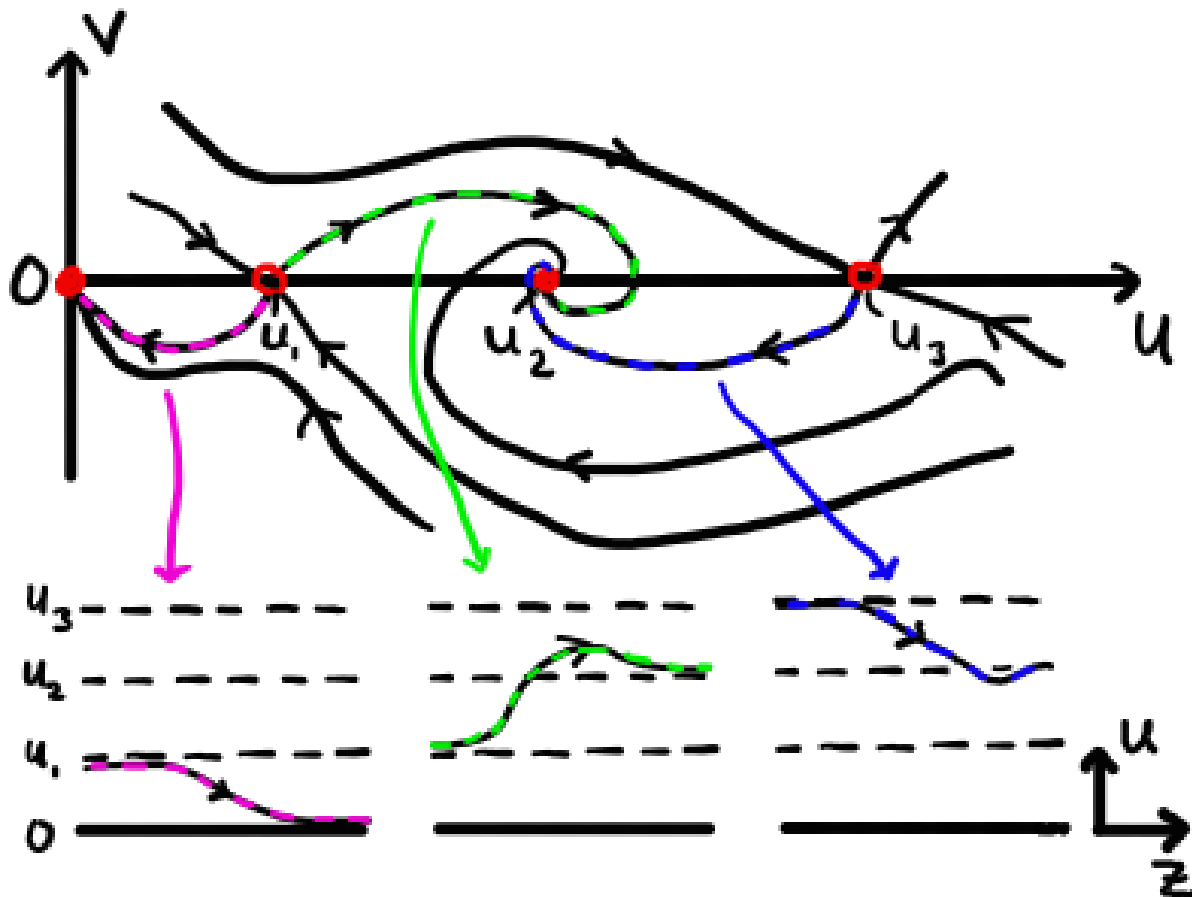
$(u^*, v^*) = (0, 0)$: stable node/spiral

$(u^*, v^*) = (u_1, 0)$: saddle point

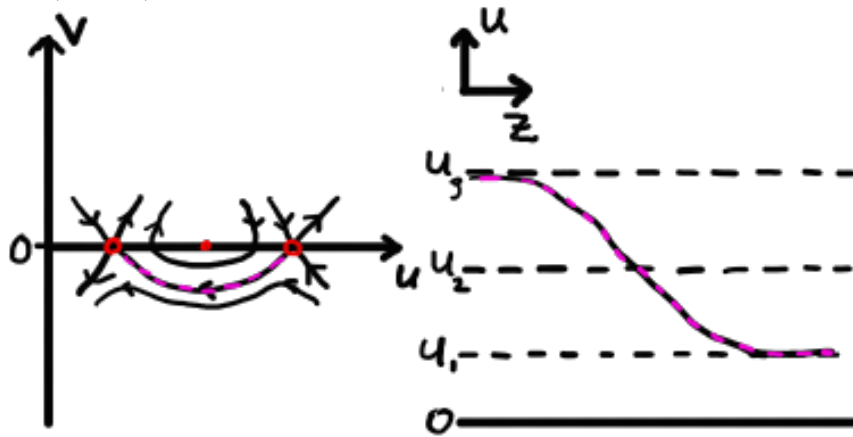
$(u^*, v^*) = (u_2, 0)$: stable node/spiral

$(u^*, v^*) = (u_3, 0)$: saddle point

The types of fixed points obtained depend on c and the system parameters. Example (origin node, $(u_2, 0)$ spiral) allows for several travelling waves (which one of these is selected depends on initial + boundary conditions):



If $(u_2, 0)$ is a center, a connection between saddles 1 and 3 is possible:



If $c > 0$ outbreak spreads (case plotted, the wave leaves a population of size u_3 in its wake), if $c < 0$ outbreak is eliminated (the wave leaves a population of size u_1).