3 Spatial Variations

In the past two sections, we considered the dynamics of functions that depend only on time. But there are other dimensions in our universe and these too can be important in biology. If, for example, you're a rabbit then the location of a fox is important to you. The purpose of this section is to include the effects of spatial localisation in our models.

Mathematically, this means that our variables depend both on time t and on space $\mathbf{x}$. For example, instead of working with a total population $N(t)$, we instead have a *population density* $n(\mathbf{x}, t)$. If you integrate this density over some region V then it tells you the total population inside that region

$$N(t) = \int_V d^3x \; n(\mathbf{x}, t) \; . \tag{3.1}$$

The fact that we're dealing with functions of space and time means that our system will no longer be described by a system of ordinary differential equations. Instead, we must embrace partial differential equations and all they have to offer.

The Continuity Equation

Many of the variables of interest in mathematical biology are counting things. And these things are, by and large, conserved.

That sentence may seem strange given that everything we've done so far is devoted to understanding the time evolution of these variables. If they were truly conserved then they wouldn't change! But, as a starting point, the conservation of things is important. For example, it's true that you were born and you will die but, if you're lucky, there's a good 70 to 80 years in between in which neither of these things happens. This means that the population is approximately conserved. We can then start to look at how birth and death rates change this conclusion.

Crucially, when things are conserved in physics (and, indeed, in biology) they are conserved *locally*. The amount of conserved quantity can change in one region of space, but only because it moves to a neighbouring region. There is an important and ubiquitous equation that captures this fact: the density of some stuff $n(\mathbf{x}, t)$ is conserved if there exists a vector function $\mathbf{J}(\mathbf{x}, t)$, known as a *current density* or *flux*, that obeys

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = 0 \; . \tag{3.2}$$

This is the *continuity equation*. We've met it previously in courses on Electromagnetism (where electric charge is conserved), Fluid Mechanics (where mass is conserved), and Quantum Mechanics (where probability is conserved).

To see why the continuity equation (3.2) implies conservation, we integrate both sides over a region of space V with boundary $S = \partial V$ and then invoke Gauss' divergence theorem,

$$\frac{dN}{dt} = \int_V d^3x \, \frac{\partial n}{\partial t} = -\int_V d^3x \, \nabla \cdot \mathbf{J} = -\int_S d^2\mathbf{S} \cdot \mathbf{J} \ . \tag{3.3}$$

We learn that the total population $N(t)$ in some region V can change with time, but only if there is a flux of the current $\mathbf{J}$ out of the boundary of the region. Often we will be interested in some closed region V from which there is no escape.In this case we have $\mathbf{J} = 0$ on the boundary S and, correspondingly, N is constant. For convenience, we may sometimes, unrealistically in the context of biology, take $V = \mathbb{R}^3$ and require that $\mathbf{J} \to 0$ suitably fast asymptotically.

Anything that is conserved obeys the continuity equation (3.2). But, as we have stressed, our populations and other beasts are typically not fully conserved. In this case, it's straightforward to amend the continuity equation: we just include an additional term on the right-hand side

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = F(\mathbf{x}, t) \ . \tag{3.4}$$

This function $F(\mathbf{x}, t)$ captures any loss or creation of the quantity of interest. For example, if $n(\mathbf{x}, t)$ is the population density then $F(\mathbf{x}, t)$ may describe the birth and death rates, now allowed to vary in both space and time. The function F may itself depend on n or (less commonly) $\mathbf{J}$.

Local conservation means that it's not enough to talk only about the density $n(\mathbf{x}, t)$: we also need to introduce the current density $\mathbf{J}(\mathbf{x}, t)$. In general, this could be an independent variable. But there are two situations that arise most commonly:

- Diffusion: When the underlying density is subject to constant, random fluctuations, the result is that the current is given by

  $$\mathbf{J}(\mathbf{x}, t) = -D\nabla n(\mathbf{x}, t) \ . \tag{3.5}$$

  This is known as *Fick's law* and D is a constant known as the *diffusivity*. Fick's law is telling us that there is a current from high density regions to low density

regions. We will get more intuition for this result in Section 4 when we discuss the effects of randomness and, in particular, when we derive the Fokker-Planck equation. For now, we will take this result as an assumption and see where it takes us. With a current of this form, the continuity equation becomes

$$\frac{\partial n}{\partial t} = D\nabla^2 n \ . \tag{3.6}$$

This is the *heat equation*. Processes governed by this equation are said to undergo *diffusion*. We will devote Section 3.1 to solving this equation. For now, note that this equation makes it clear that the dimension of the diffusivity is $[D] = L^2/T$.

- Advection: An alternative scenario is that the stuff we care about is sitting in some moving, background medium and just going with the flow. In this case, the current is given by

$$\mathbf{J}(\mathbf{x}, t) = n(\mathbf{x}, t)\, \mathbf{u}(\mathbf{x}, t) \tag{3.7}$$

where $\mathbf{u}(\mathbf{x}, t)$ is the underlying velocity field. This kind of current typically arises in fluid mechanics and is known as *advection*. In this case, you need to separately specify the form of the velocity field or, if it's a dynamical variable, introduce more equations (such as the Euler or Navier-Stokes equations) that govern its properties.

In general, it's quite possible that the current has both a diffusive piece and an advective piece.

In both the examples above, there can be no current $\mathbf{J}(\mathbf{x}, t)$ if $n(\mathbf{x}, t) = 0$. That's in contrast to what happens in electromagnetism where it's quite possible to have $\mathbf{J} =\neq 0$ even if the charge density $n = 0$. That's because electromagnetism comes with both positive and negative charges which cancel out. But if the negative charges move, while the positive charges stay still – which is what happens in a wire conducting electricity – then the current is non-zero. In contrast, the diffusion and advection described above typically happens in situations where $n(\mathbf{x}, t) > 0$. This, of course, is the situation for populations.

There are other ways to generalise the ideas above, some of which we will meet later. For example, the diffusivity D in (3.5) could depend on the function $n(\mathbf{x}, t)$. The same is true of the forcing function F in (3.4). If we have standard diffusion, together with a field-dependent forcing $F(n)$, we are left with a class of equations that take the form

$$\frac{\partial n}{\partial t} - D\nabla^2 n = F(n) \ . \tag{3.8}$$

These are known as *reaction-diffusion equations*, with the $D\nabla^2 n$ term capturing diffusion and the $F(n)$ term said to be the "reaction". This is the class of equations that we will mostly focus on in this section.

3.1 Diffusion

We first study the solutions to the heat equation (3.6) in various situations. To keep things simple, we will restrict ourselves to the one-dimensional case,

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} \ . \tag{3.9}$$

As we proceed, we'll also look at some generalisations of this equation.

3.1.1 Diffusion on a Finite Interval

We start by placing our system on a finite interval $x \in [0, L]$. We will impose boundary conditions on both ends

$$n(0,t) = n_0 \quad \text{and} \quad n(L,t) = n_1 \ . \tag{3.10}$$

with n_0 and n_1 both constant. In the context of thermodynamics, we might think of $n(x,t)$ as the temperature along a one-dimensional rod with the two ends sitting in some heat reservoir, held at fixed temperatures. In the context of biology, we could think of $n(x,t)$ as the population of something small (say, an ant or a bacterium) which can move along a narrow tube. The ends of the tube are connected to two population reservoirs, each held at constant population density. The heat equation (3.9) then tells us how the temperature/population varies along the tube.

To start, we can look for a steady state solution with no time dependence. This is straightforward. We have

$$\frac{\partial^2 n}{\partial x^2} = 0 \quad \Longrightarrow \quad n(x,t) = n^\star(x) = n_0 + (n_1 - n_0)\frac{x}{L} \tag{3.11}$$

where we've implemented the boundary conditions (3.10). We've called this solution $n^\star(x)$ because it's analogous to the fixed points that we found in the dynamical systems of Section 1.

For this steady state, the flux is $J = -D\,\partial n/\partial x = D(n_0 - n_1)/L$ is constant. If $n_0 > n_1$ then $J > 0$. If $n_0 < n_1$ then $J < 0$. In both cases, there is a net flux from the high density population to the low density population.

As we mentioned briefly above (and will see more in Section 4), diffusion typically happens where there is some underlying randomness in the situation. Having a net flux $J > 0$ doesn't mean that the ants are marching in lockstep from left to right. There may be some ants wandering in one direction and some in the other. But there's an overall preference for them to travel left to right. Our diffusion model doesn't capture these microscopic fluctuations: only the overall trend of the flow.

Time Dependence

What happens when we deviate from the steady state? Now we need to specify the initial value of the field at $t = 0$. The resulting solution takes the form

$$n(x, 0) = n^\star(x) + c(x, t) \ . \tag{3.12}$$

where $c(x, t)$ also solves the heat equation

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \tag{3.13}$$

now with boundary conditions $c(0, t) = c(L, t) = 0$.

We can look for separable solutions of the form

$$c(x, t) = f(x)\, g(t) \ . \tag{3.14}$$

Substituting this into the heat equation, we see that the two functions must obey

$$f\dot{g} = Dgf'' \ . \tag{3.15}$$

Dividing through by fg, we have

$$\frac{\dot{g}}{g} = D\frac{f''}{f} \ . \tag{3.16}$$

But the left-hand side is a function only of t, and the right-hand side is a function only of x, which means that actually both sides must be constant. The solution for $f(x)$ is constrained by the boundary conditions $f(0) = f(L) = 0$ which tells us that solutions must be of the form

$$f''(x) \propto f(x) \quad \Longrightarrow \quad f(x) = \sin\left(\frac{\pi n x}{L}\right) \quad \text{with} \quad n = 1, 2 \ldots \tag{3.17}$$

Now (3.16) fixes the form of $g(t)$,

$$\dot{g} = -\lambda_n g \quad \Longrightarrow \quad g = e^{-\lambda_n t} \quad \text{with} \quad \lambda_n = \frac{D\pi^2 n^2}{L^2} \ . \tag{3.18}$$

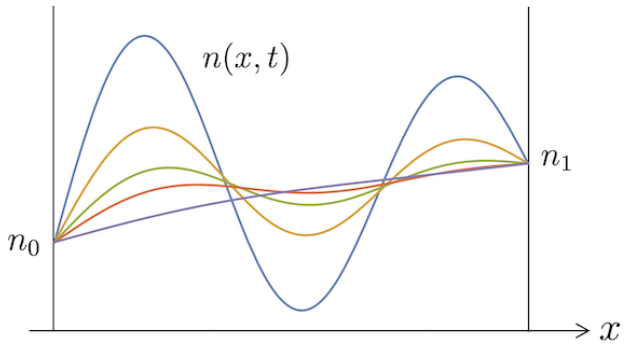


Figure 39. Diffusion of an initial wiggly profile quickly settles down to the linear, steady state.

Because the heat equation is linear, we can simply add together separable solutions for different n. Moreover, the most general solution can be constructed in this way and takes the form

$$c(x,t) = \sum_{n=1}^{\infty} c_n e^{-\lambda_n t} \sin\left(\frac{\pi n x}{L}\right) \ . \tag{3.19}$$

Here the c_n are determined by the initial conditions where they are essentially Fourier components of the initial profile at time $t = 0$. We now see the key feature of the heat equations: all the higher Fourier modes die off exponentially quickly, tending towards the steady state solution. The higher the Fourier mode, so the more wiggly the profile, the faster it decays away. This is the characteristic behaviour of the heat equation: it smooths things out. An example of the evolution of $n(x,t)$, plotted for increasing values of t is shown in Figure 39.

No Flux Boundary Condition

We can look at generalisations of this set-up. For example, instead of fixing the value of $n(x,t)$ on both ends, we could instead require that, say, $n(0,t) = n_0$ on the far left, but

$$J = -D\frac{\partial n}{\partial x} = 0 \ . \tag{3.20}$$

on the far right at $x = L$. Mathematically we say that we are imposing Dirichlet boundary conditions on the left, and Neumann boundary conditions on the right. Physically, we might have a tube connected to a population of ants but, having travelled all the way down it, the ants are disappointed to find that the end is closed off, ensuring that there is no flux.

Now the steady state solution is simply $n(x,t) = n_0$ and we can again write the most general solution as $n(x,t) = n_0 + c(x,t)$. We can proceed largely as before, looking first for separable solutions of the form $n(x,t) = f(x)\,g(t)$ which must obey (3.16). The novelty now comes in the boundary conditions that are imposed on $f(x)$ which hold if we take

$$f(x) = \sin\left(\frac{(2n-1)\pi x}{2L}\right) \quad . \quad \text{with} \quad n = 1, 2, \ldots \tag{3.21}$$

The most general solution is then

$$n(x,t) = n_0 + \sum_{n=1}^{\infty} c_n e^{-\lambda_n t} \sin\left(\frac{(2n-1)\pi x}{2L}\right) \quad . \quad \text{with} \quad \lambda_n = \frac{D(2n-1)^2\pi^2}{4L^2} \quad . \tag{3.22}$$

Again, we see the key feature: the faster the wiggle, the faster they die out.

3.1.2 How to Cook a Turkey

If you buy a turkey, the instructions will typically tell you to cook it for 20 minutes per kg, and then another 70 minutes for a 2-4 kg turkey, or another 90 minutes for a 4-10 kg turkey. These slightly convoluted rules arise because the relationship between the cooking time and the weight is not linear. The correct relationship was suggested by the particle physicist Pief Panofsky who pointed out that the cooking time τ scales with the mass M by the relation

$$\tau \sim M^{2/3} \; . \tag{3.23}$$

We can derive this formula using the ideas of diffusion described above[8].

The temperature $T(\mathbf{x}, t)$ of the turkey is described by the heat equation, now in 3d

$$\frac{\partial T}{\partial t} = D\nabla^2 T \; . \tag{3.24}$$

In fine tradition, we will assume that our turkey is spherical. (The analysis below also holds for spherical cows.) Then, further assuming that the oven is also spherically symmetric we can think of $T = T(r,t)$ with r the radial coordinate and the heat equation takes the form

$$\frac{\partial T}{\partial t} = \frac{D}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) \quad . \tag{3.25}$$

[8]This is taken from the paper Physics in Turkey Cooking by Jin, Wang and Wang. I'm grateful to Ray Goldstein for pointing me to this paper.

At this point, we use a trick and write $V(r,t) = rT(r,t)$. (We used a similar trick in the lectures on Quantum Mechanics when solving the Schrödinger equation in 3d.) Then we have $T' = V'/r - V/r^2$ and, rather wonderfully, the heat equation becomes

$$\frac{\partial V}{\partial t} = D\frac{\partial^2 V}{\partial r^2} \ . \tag{3.26}$$

We see that, in this new variable V, we're back solving the 1d diffusion equation. And we know how to do that! A separable solution takes the form

$$V(r,t) = e^{-\lambda Dt}\big[A\cos(\sqrt{\lambda}r) + B\sin(\sqrt{\lambda}r)\big] \ . \tag{3.27}$$

for some $\lambda > 0$. The temperature T is given by $T = V/r$ so if we want to avoid a divergence at $r = 0$ then we need to set $A = 0$. Our solution will involve only $\sin(\sqrt{\lambda}r)$.

We can determine the allowed values of λ, together with the constants A and B, by looking at the boundary conditions. If the turkey has radius R, then we have the boundary condition

$$T(r,t) = T_{\rm hot} \quad \text{for all } t \text{ and } r \geq R \tag{3.28}$$

Here $T_{\rm hot}$ is the temperature of the oven. This is telling us that we can deviate from the uniform temperature only inside the turkey, $r < R$. We do this by taking $\sqrt{\lambda} = n\pi/R$ with $n \in \mathbb{Z}^+$ and writing down the general solution

$$T(r,t) = T_{\rm hot} + \frac{1}{r}\sum_{n=1}^{\infty}\left[V_n \sin\left(\frac{n\pi r}{R}\right) e^{-n^2\pi^2 Dt/R^2}\right] \ . \tag{3.29}$$

The coefficients V_n are set by the initial conditions. We'll take this to be

$$T(r,0) = T_0 \ll T_{\rm hot} \quad \text{for} \quad 0 \leq r < R \tag{3.30}$$

This initial data is discontinuous at $r = R$ where the temperature jumps from T_0 to $T_{\rm hot}$, but it's straightforward to implement this. We just need to pick the coefficients V_n so that that it gives the Fourier decomposition of a linear function r, cancelling the $1/r$ in the denominator. It's simple to check that this is achieved by the solution

$$T(r,t) = T_{\rm hot} - \frac{2R}{\pi^2}\frac{(T_{\rm hot} - T_0)}{r}\sum_{n=1}^{\infty}\left[\frac{(-1)^n}{n}\sin\left(\frac{n\pi r}{R}\right) e^{-n^2\pi^2 Dt/R^2}\right] \ . \tag{3.31}$$

These initial conditions decay away in characteristic time

$$\tau = \frac{R^2}{n^2\pi^2 D} \ . \tag{3.32}$$

When the lowest $n = 1$ mode has decayed away, the turkey is cooked, approaching the steady state solution $T(r,t) = T_{\rm hot}$. Importantly, $\tau \sim R^2$. This is the origin of the Panofsky turkey rule (3.23), since the mass is proportional to volume $M \sim R^3$.

To put some numbers of this, we need to know the diffusivity for heat in a turkey. That can be easily measured to be $D \approx 2 \times 10^{-3}$ cm^{2}s^{-1}. Suppose that our turkey has radius $R \approx 10$ cm, then we find $\tau \approx 5000$ seconds, or about 80 minutes. You might want to wait for, say $2 \times \tau$, to be convinced that you're not going to get salmonella, so pop it in for three hours and voilà. Don't let anyone tell you that maths isn't useful.

3.1.3 A First Look at Diffusion With Growth

In preparation for more interesting things to come (noticeably, the Turing instability) we can look at what happens if we deform the heat equation. We will take our substance to diffuse, but now with a linear growth term on the right-hand side

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} + \lambda n \tag{3.33}$$

with k constant.

We'll again take the system on an interval $x \in [0, L]$ and we'll take the simple situation where we impose boundary condition $n(0,t) = n(0,L) = 0$. If there was no growth term, then the system would settle down to the empty state $n = 0$. Conversely, if there was no diffusion, so $D = 0$, then we know that the population n will grow exponentially quickly. In combining the two terms we have introduced what story tellers call narrative tension. Something interesting should now happen.

There is a trick to solving this equation. We define a new variable

$$\tilde{n}(x,t) = e^{-\lambda t} n(x,t) \quad \Longrightarrow \quad \frac{\partial \tilde{n}}{\partial t} = D\frac{\partial^2 \tilde{n}}{\partial t^2} \ . \tag{3.34}$$

We see that this new variable solves our original heat equation. We can just import our previous solution (3.19) to find

$$n(x,t) = \sum_{n=1}^{\infty} c_n e^{(\lambda - \lambda_n)t} \sin\left(\frac{\pi n x}{L}\right) \quad \text{with} \quad \lambda_n = \frac{D\pi^2 n^2}{L^2} \ . \tag{3.35}$$

Although the maths was straightforward, the resulting physics is novel. There is a critical length of the interval

$$L_c = \sqrt{\frac{D\pi^2}{\lambda}} \ . \tag{3.36}$$

For $L < L_c$, the system settles down to the boring steady state $n = 0$ where everything diffuses out the end points. But for suitably long intervals, $L > L_c$, the system becomes unstable with the lowest $n = 1$ mode the first to start growing. As we make L yet longer, successive modes also become unstable.

The idea that adding an additional term to the diffusion equation can lead to spatial instability is something that we will see again shortly.

3.1.4 Diffusion on the Line

The boundary conditions played a crucial role in constructing the solutions above. What happens if we want to solve the heat equation

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} \tag{3.37}$$

on an infinite line?

We will insist that our density is localised somewhere (say, near the origin) and, moreover that $J \sim \partial n/\partial x \to 0$ as $x \to \pm\infty$. This then ensures that the total amount of stuff

$$N = \int_{-\infty}^{+\infty} dx\ n(x,t) \tag{3.38}$$

is constant, with

$$\frac{dN}{dt} = \int_{-\infty}^{+\infty} dx\ \frac{\partial n}{\partial t} = D\int_{-\infty}^{+\infty} dx\ \frac{\partial^2 n}{\partial x^2} = D\left[\frac{\partial n}{\partial x}\right]_{-\infty}^{+\infty} = 0\ . \tag{3.39}$$

We won't give the most general solution to the heat equation. Instead, we will find a particular solution that is "self-similar", meaning that after scaling space and time in a certain way, it looks the same.

The essence of these self-similar solutions is that we can replace the partial differential equation (3.37) with an appropriate ordinary differential equation, where the relevant variable is a suitable combination of x and t. To figure out what linear combination works, we do a little dimensional analysis.

We have two variables x and t and two constants with dimension $[D] = L^2T^{-1}$ and $[N] = L$. (Here we're assuming that $n(x,t)$ itself is dimensionless; you could assign it a dimension of "people density" or "bugs density" or whatever, but this won't change the conclusions below). We then introduce the dimensionless combination

$$\xi = \frac{x}{\sqrt{Dt}}\ . \tag{3.40}$$

Furthermore, we look for solutions of the form

$$n(\mathbf{x},t) = \frac{N}{\sqrt{Dt}}\, f(\xi)\ . \tag{3.41}$$

The idea here is that the constant N sets the overall scale of the solution and the factor of $(Dt)^{-1/2}$ ensures that the function $f(\xi)$ is dimensionless. At this point we have to roll up our sleeves and figure out what the heat equation looks like when written in terms of ξ. We have

$$\frac{\partial \xi}{\partial t} = -\frac{1}{2}\frac{\xi}{t} \quad \text{and} \quad \frac{\partial \xi}{\partial x} = \frac{1}{\sqrt{Dt}} = \frac{\xi}{x} \ . \tag{3.42}$$

The time derivative of $n(x,t)$ is then

$$\begin{aligned} \frac{\partial n}{\partial t} &= -\frac{1}{2t}\frac{N}{\sqrt{Dt}} f + \frac{N}{\sqrt{Dt}} f'(\xi)\frac{\partial \xi}{\partial t} \\ &= -\frac{1}{2t}\frac{N}{\sqrt{Dt}}(f + \xi f') \\ &= -\frac{1}{2t}\frac{N}{\sqrt{Dt}}\frac{d}{d\xi}(\xi f) \ . \end{aligned} \tag{3.43}$$

Meanwhile, the spatial derivatives are

$$\frac{\partial}{\partial x} = \frac{1}{\sqrt{Dt}}\frac{\partial}{\partial \xi} \quad \text{and} \quad \frac{\partial^2}{\partial x^2} = \frac{1}{Dt}\frac{\partial^2}{\partial \xi^2} \ . \tag{3.44}$$

Putting this together, the heat equation (3.37) becomes the ordinary differential equation

$$\frac{d^2 f}{d\xi^2} + \frac{1}{2}\frac{d}{d\xi}(\xi f) \ . \tag{3.45}$$

It's simple to integrate this once:

$$\frac{df}{d\xi} + \frac{1}{2}\xi f = \text{constant} \ . \tag{3.46}$$

If we want a localised solution, with $f, f' \to 0$ as $\xi \to \infty$ then this constant must vanish. We learn that we must solve

$$\frac{df}{d\xi} = -\frac{1}{2}\xi f \quad \Longrightarrow \quad f(\xi) = Ae^{-\xi^2/4} \ . \tag{3.47}$$

The normalisation condition (3.38) translates to the requirement

$$\int_{-\infty}^{+\infty} d\xi \ f(\xi) = 1 \quad \Longrightarrow \quad A = \frac{1}{\sqrt{4\pi}} \ . \tag{3.48}$$

The upshot of this analysis is that we have a self-similar solution to the heat equation given by

$$n(x,t) = \frac{N}{\sqrt{4\pi Dt}} e^{-x^2/4Dt} \ . \tag{3.49}$$

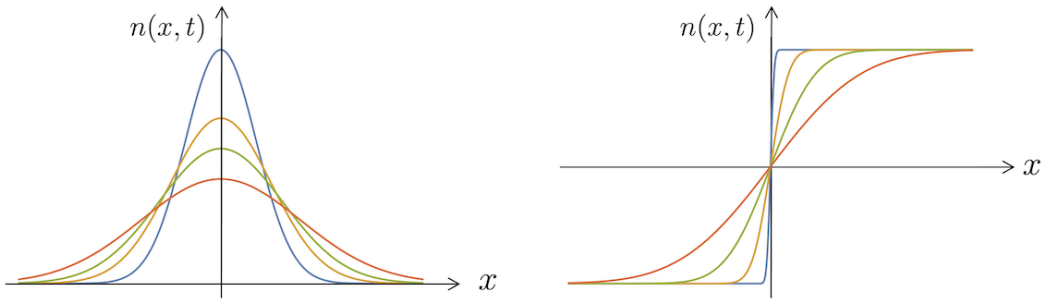


Figure 40. On the left: diffusion of a Gaussian wavepacket. On the right: diffusion of the error function. In both cases, diffusion takes the edge off.

This is a Gaussian of ever-spreading width. If we trace it back to $t \to 0^-$, it becomes a delta-function localised at the origin. Again, we see the tendency of the heat equation to take a solution and spread it out. The resulting profile for various values of t is shown on the left of Figure 40.

Changing Boundary Conditions at Infinity

We can get solutions with different boundary conditions using a slight variation of this argument. Suppose that we want a solution to the heat equation such that

$$n(x,t) \to \begin{cases} +1 & x \to +\infty \\ -1 & x \to -\infty \end{cases} . \tag{3.50}$$

Now there's no analog of the conserved quantity N because the spatial integral over $n(x,t)$ diverges. But, inspired by the approach above, we could look for solutions of the form

$$n(x,t) = t^\alpha g(\xi) \quad \text{with} \quad \xi = \frac{x}{\sqrt{Dt}} \tag{3.51}$$

and some constant α that we need to determine. The two sides of the heat equation then become

$$\frac{\partial n}{\partial t} = t^{\alpha-1}\left(\alpha - \frac{1}{2}\xi g'\right) \quad \text{and} \quad \frac{\partial^2 n}{\partial x^2} = \frac{t^\alpha}{Dt} g'' . \tag{3.52}$$

This time, the factors of t work out on both sides. But if we want to impose the boundary conditions $n(x,t) \to \pm 1$ on both sides, then we had better take $\alpha = 0$. The heat equation becomes

$$g'' + \frac{1}{2}\xi g' = 0 . \tag{3.53}$$

Again, we can integrate to get

$$g'(\xi) = Ae^{-\xi^2/4} \quad \Longrightarrow \quad g(\xi) = B + A\int_0^\xi d\eta\; e^{-\eta^2/4} \tag{3.54}$$

with A and B both integration constants. This definite integral defines the so-called *error function*

$$\text{Erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x dy\; e^{-y^2}\;. \tag{3.55}$$

It has the property that $\text{Erf}(x) \approx 2x/\sqrt{\pi}$ for $|x| \ll 1$ and $\text{Erf}(x) \to \pm 1$ as $x \to \pm\infty$. The integration constants A and B are then fixed by the boundary conditions (3.50), and we have the solution

$$n(x,t) = \text{Erf}\left(\frac{x}{\sqrt{4Dt}}\right)\;. \tag{3.56}$$

The evolution of this function with t is shown on the right-hand side of Figure 40.

Growth Revisited

We saw in Section 3.1.3 that interesting things happen if we add linear growth to the heat equation on the interval, so we have

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} + \lambda n\;. \tag{3.57}$$

Previously our interest in this came largely from the fact that there was a transition, with the growth winning when $L > L_c$ and dissipation winning when $L < L_c$. Now with L effectively infinite, you might imagine that this crossover no longer happens and growth always wins. And you would be right. For example, the dissipating Gaussian wavepacket (3.49) now solves (3.57) with

$$n(x,t) = \frac{N}{\sqrt{4\pi Dt}}e^{\lambda t}e^{-x^2/4Dt}\;. \tag{3.58}$$

For any fixed value of x, the height of the wavepacket grows exponentially in time for $\lambda > 0$. It shrinks for $\lambda < 0$.

Note that our solution (3.58) doesn't take the form $n(x,t) = t^\alpha g(x/t^\beta)$ that we would look for in a similarity solution. Indeed, you can check that no such solution of this form exists. Repeating the steps that we took above, we would end up having to solve

$$t^{\alpha-1}(\alpha g = \beta\xi g') = t^{\alpha-2\beta}Dg'' + \lambda t^\alpha g \tag{3.59}$$

and there's no way to pick α and β so that this holds for all t. This, it turns out, is rather typical: similarity solutions rarely exist when we try to solve equations with three of more terms.

3.1.5 Non-Linear Diffusion

In all the examples above, we have taken the diffusivity D to be constant. But that's not necessarily the case. In general, we could have a current given by

$$\mathbf{J} = -D(n; \mathbf{x}, t)\nabla n \tag{3.60}$$

where, as shown, D can vary over space and time or even depend on $n(\mathbf{x}, t)$ itself. Here we look at the latter situation. We will consider a diffusivity given by

$$D = k\, n(\mathbf{x}, t) \tag{3.61}$$

with $k > 0$ constant. This means that diffusion is greater when the population density is greater. It's as if the individuals are keen to get away from each other.

We again restrict ourselves to one spatial dimension. The continuity equation now gives the non-linear diffusion equation

$$\frac{\partial n}{\partial t} = -\frac{\partial J}{\partial x} = k\frac{\partial}{\partial x}\left(n\frac{\partial n}{\partial x}\right) \ . \tag{3.62}$$

As before, we can look for self-similar solutions that depend only on a single dimensionless combination of x and t. This time, however, the dimensions of our constants are different. In addition to length L and time T, we'll also need the dimension of $n(x, t)$ which, quite reasonably, we'll denote as n.

The two constants in the game are k and, provided that $J \to 0$ as $x \to \pm\infty$, the total population

$$N = \int_{-\infty}^{+\infty} n(x, t) \ . \tag{3.63}$$

These have dimensions

$$[k] = L^2T^{-1}n^{-1} \quad \text{and} \quad [N] = nL \ . \tag{3.64}$$

From these, we see that to construct a dimensionless variable proportional to x, we must take

$$\xi = \frac{x}{(Nkt)^{1/3}} \ . \tag{3.65}$$

We then take the ansatz

$$n(x, t) = \frac{N}{(Nkt)^{1/3}} f(\xi) \tag{3.66}$$

where the overall factor is designed so that $f(\xi)$ is a dimensionless function.

By now, the path should be a familiar one. We have

$$\frac{\partial \xi}{\partial t} = -\frac{1}{3}\frac{\xi}{t} \quad \text{and} \quad \frac{\partial \xi}{\partial x} = \frac{1}{(Nkt)^{1/3}} = \frac{\xi}{x} \ . \tag{3.67}$$

The time derivative of $n(x,t)$ is then

$$\begin{aligned} \frac{\partial n}{\partial t} &= -\frac{1}{3t}\frac{N}{(Nkt)^{1/3}} f + \frac{N}{(Nkt)^{1/3}} f'(\xi)\frac{\partial \xi}{\partial t} \\ &= -\frac{1}{3t}\frac{N}{(Nkt)^{1/3}}\frac{d}{d\xi}(\xi f) \ . \end{aligned} \tag{3.68}$$

Meanwhile, the first spatial derivative is

$$\frac{\partial n}{\partial x} = \frac{N}{(Nkt)^{2/3}} f'(\xi) \tag{3.69}$$

and so the combination in (3.62) becomes

$$\frac{\partial}{\partial x}\left(n\frac{\partial n}{\partial x}\right) = \frac{1}{(Nkt)^{1/3}}\frac{\partial}{\partial \xi}\left(\frac{Nf}{kt}\frac{df}{d\xi}\right) = \frac{1}{kt}\frac{N}{(Nkt)^{1/3}}\frac{d}{d\xi}(ff') \ . \tag{3.70}$$

Putting these together, the non-linear diffusion equation (3.62) becomes

$$\frac{d}{d\xi}(ff') = -\frac{1}{3}\frac{d}{d\xi}(\xi f) \quad \Longrightarrow \quad ff' = -\frac{1}{3}\xi f \tag{3.71}$$

where we've eliminated an integration constant by requiring that $f, f' \to 0$ as $x \pm \infty$.

We see that we have two different solutions. The first is $f = 0$, which is rather boring. The second is

$$f' = -\frac{\xi}{3} \quad \Longrightarrow \quad f = -\frac{\xi^2}{6} + \text{constant} \ . \tag{3.72}$$

That looks more interesting but, sadly, it doesn't satisfy our boundary conditions $f \to 0$ as $\xi \to \pm\infty$.

What's going on?! We've got one nice quadratic solution that doesn't satisfy the boundary conditions, and one boring solution $f = 0$ that doesn't satisfy the fact that total population is a constant N. Indeed, it's simple to check that the integral (3.63) translates to an integral of $f(\xi)$,

$$\int_{-\infty}^{+\infty} d\xi \ f(\xi) = 1 \ . \tag{3.73}$$

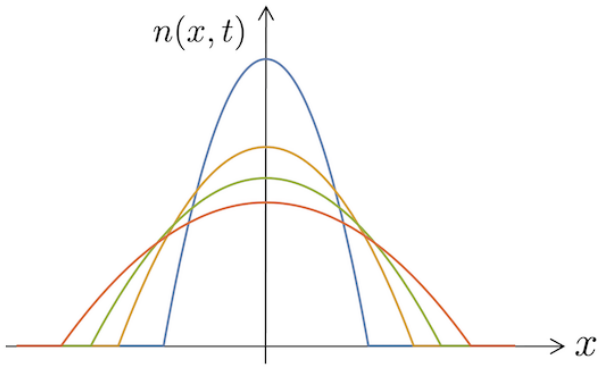


Figure 41. The non-linear diffusion equation results in this weird portion of a parabola expanding outwards.

We can make progress by splicing together these two solutions. We take

$$f(\xi) = \begin{cases} A - \xi^2/6 & |\xi| < \xi_0 = \sqrt{6A} \\ 0 & |\xi| \geq \xi_0 \end{cases} \tag{3.74}$$

The crossover ξ_0 is chosen so that the function is continuous (and, moreover, so that $f(\xi)$ is everywhere non-negative). The derivative of the $f(\xi)$ is discontinuous at ξ_0 and we should really work a little harder to show that this kind of splicing is allowed. The reason it's acceptable can be traced to the condition $f(f' - \xi/3) = 0$ in (3.71) with, roughly speaking, the $f = 0$ beating the fact that f' isn't well-defined at the splice. In particular, the current $J \sim ff'$ vanishes at the point $\xi = \pm\xi_0$. In the mathematics literature, these are sometimes called *weak solutions*, which means that they can be shown to satisfy the original equation in some well-defined sense.

The constant A is fixed by the normalisation condition (3.73),

$$1 = \int_{-\xi_0}^{\xi_0} d\xi \; f(\xi) = 2A\xi_0 - \frac{1}{9}\xi_0^3 = \frac{4\sqrt{6}}{3}A^{3/2} \; . \tag{3.75}$$

This gives $A = (3/32)^{1/3}$ and $\xi_0 = \sqrt{6A} = (9/2)^{1/3}$. This then gives us our final result: going back to the x and t variables, the density $n(x,t)$ takes the shape of finite piece of parabola, spreading out over time

$$n(x,t) = \frac{1}{6}\frac{N^{2/3}}{(kt)^{1/3}}\left[\left(\frac{9}{2}\right)^{2/3} - \frac{x^2}{(Nkt)^{2/3}}\right] \quad \text{for} \quad x < \left(\frac{9}{2}Nkt\right)^{1/3} \; . \tag{3.76}$$

with $n(x,t) = 0$ outside this region. The result is shown in Figure 41.

The end result is slightly odd, not least because we have come to expect that sharp edges are washed out by diffusion, but here the corner at $n(x,t) = 0$ persists for all time. This is a novelty that comes from the non-linear aspect of diffusion. In particular, we have $D \sim n$ so it's not possible for the system to diffuse when $n = 0$. Instead, the population piles up near the edges and, as it grows, diffuses faster.

3.2 Travelling Waves

Once we have both diffusion and some forcing term, interesting things can happen. Before we get to the interesting things, let's look at some boring things.

The one-dimensional reaction-diffusion equation takes the form

$$\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2} + F(n) \tag{3.77}$$

for some "reaction" forcing function $F(n)$. An obvious way to proceed is to look for spatially homogeneous solutions, with $n(x,t) = n(t)$. Then the equation becomes

$$\frac{\partial n}{\partial t} = F(n) \ . \tag{3.78}$$

But this is precisely the kind of equation that we started exploring in Section 1. And with just a single variable $n(t)$, there's not a great deal that can happen. We look for fixed points $n^\star$ that obey

$$F(n^\star) = 0 \ . \tag{3.79}$$

Now we can look at perturbations around this fixed point. The novelty is that these perturbations need not be spatially homogeneous: we write

$$n(x,t) = n^\star + \epsilon(x,t) \ . \tag{3.80}$$

Substituting this into (3.77), we get a reaction-diffusion equation for $\epsilon(x,t)$,

$$\frac{\partial \epsilon}{\partial t} = D\frac{\partial^2 \epsilon}{\partial x^2} + \lambda\epsilon \quad \text{with} \quad \lambda = \frac{\partial F}{\partial n}(n^\star) \ . \tag{3.81}$$

But this is the diffusion with linear growth that we already studied in Section 3.1. If we're studying the equation on the domain $x \in \mathbb{R}$ then things are particularly straightforward: the perturbation grows if $\lambda > 0$ and decays if $\lambda < 0$. (If we're instead working on an interval then, as we saw in Section 3.1.3, there is a phase transition in the behaviour as we vary the length of the interval.)

The real interest occurs when the system is unstable because the perturbative analysis above quickly breaks down and fails to tell us what really happens. In this section, we will explore some important examples of reaction-diffusion equations and see some of the novel things that can occur. A recurring lesson will be that non-linear PDEs like (3.77) can offer a much richer experience than boring linear PDEs like (3.81).

3.2.1 The KPP-Fisher Equation

The first non-linear dynamical system that we explored in Section 1 was the logistic equation. That too will be our first non-linear PDE. We will call the dimensionless dynamical variable $p(x,t)$ (rather than $n(x,t)$) and consider the 1d reaction-diffusion equation

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2} + p(1-p) \ . \tag{3.82}$$

This is the *KPP-Fisher equation*, with the initials reflecting the important work done by Kolmogorov, Petrovsky and Piskunov.

Fisher originally introduced this equation in 1937 to describe the spread of advantageous genes, with $p(x,t)$ the percentage of the population that carries the gene[9]. We already saw in Section 1.1.2 that the logistic equation describes the spread of a beneficial mutation. The novelty here is the diffusion term which captures how this beneficial mutation evolves in space.

The logistic equation has two fixed points: $p = 0$ and $p = 1$. The latter is stable, the former unstable. The question that we would like to ask is: suppose that we start at $p = 0$ and then perturb the system with a spatially localised disturbance, like the alpha variation of COVID-19 kicking off in Kent. How does it subsequently propagate?

Here is a guess. Suppose that we start with a small disturbance, localised in a region of size L around $x = 0$ at time $t = 0$. From what we've learned about diffusion and growth, we might expect that this perturbation will grow in both height and width, with the top plateauing at the fixed point $p = 1$. If we're sitting at some distance $x \ll L$ from the initial perturbation, we have to wait some time until this perturbation hits us. A cartoon of this dynamics is shown in Figure 42.

[9]The paper is "The wave of advance of advantageous genes", published in the queasily named Annals of Eugenics.

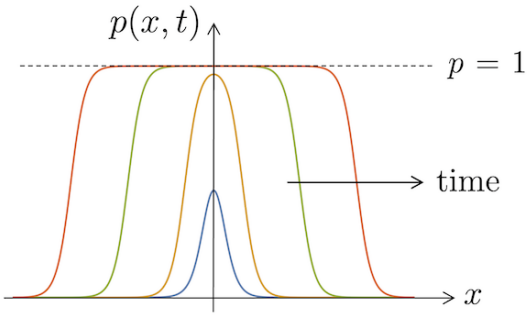


Figure 42. A cartoon of the evolution of a small perturbation in the Fisher equation, spreading out over time as a wavefront.

This suggests that we might look for wave-like solutions to the KPP-Fisher equation. It's worth pointing out that we're not guaranteed that such solutions exist. Indeed, the basic diffusion equation does not support wave-like solutions. But the addition of a reaction term changes the story and, as we'll now show, such waves typically do exist.

We don't know how fast such a wave travels so we'll leave this as arbitrary for now and call it c. We will then look for solutions of the form

$$p(x,t) = f(\xi) \quad \text{with} \quad \xi = x - ct \tag{3.83}$$

with $c > 0$ the as yet unknown wave speed. We don't know if such a solution exists, but it seems like a reasonable place to look. If we substitute this into the Fisher equation, we get an ordinary differential equation

$$-cf' = f'' + f(1-f) \ . \tag{3.84}$$

Our task is to analyse solutions to this equation. Here we offer a number of ways to do this.

Phase Plane Analysis

To start, we can turn our second order differential equation into a pair of first order differential equations,

$$f' = g \quad \text{and} \quad g' = -cg - f(1-f) \ . \tag{3.85}$$

This is the kind of system that we became adept at solving in Section 1 and we know the drill by now. First we look for fixed points. There are two $(f,g) = (0,0)$ and $(f,g) = (1,0)$.

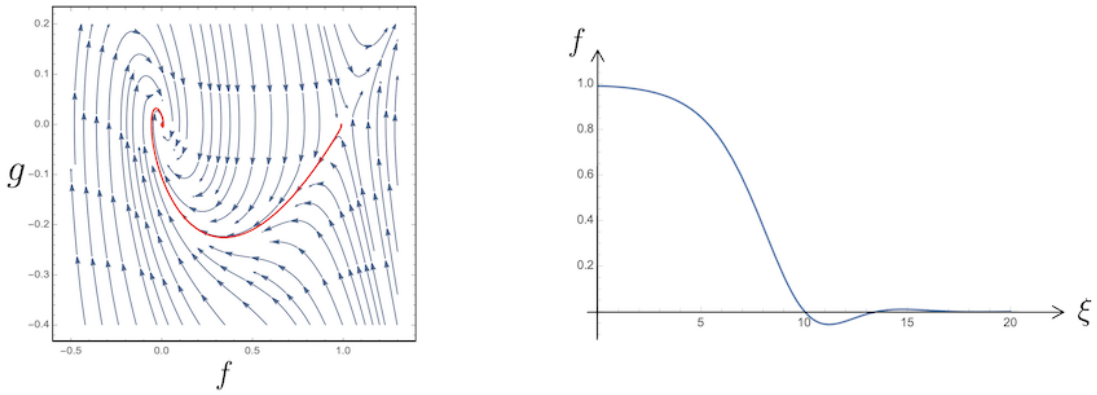


Figure 43. Numerical solutions with $c = 1$, both in the phase plane (on the left) and the evolution of $f(\xi)$. The red line shows the trajectory of a solution that starts close to the unstable fixed point $(f, g) = (1, 0)$.

Next we look at stability. The Jacobian is

$$J = \begin{pmatrix} 0 & 1 \\ -1 + 2f & -c \end{pmatrix} . \tag{3.86}$$

For $(f, g) = (1, 0)$, we have $\det J = -1$ and $\mathrm{Tr}\, J = -c$ so this fixed point is necessarily a saddle.

The other fixed point at $(f, g) = (0, 0)$ is more interesting. The eigenvalues λ of the Jacobian are

$$\lambda^2 + c\lambda + 1 = 0 \quad \Longrightarrow \quad \lambda = -\frac{c}{2} \pm \frac{1}{2}\sqrt{c^2 - 4} \, . \tag{3.87}$$

For $c < 2$, the eigenvalues are complex, with negative real part, so the fixed point is a stable focus, with trajectories spiralling in. For $c \geq 2$, the eigenvalues are real and negative (strictly, one vanishes when $c = 2$) and so the fixed point is stable.

The fact that the flows in the phase plane have qualitatively different behaviour for $c < 2$ and $c > 2$ is important. In particular, we can look at the kind of solutions we get with $c < 2$. These are plotted numerically in Figure 43. While these are fine formal solutions to the Fisher equation, because they spiral into the origin they necessarily have a region of ξ for which $f < 0$. But if we're thinking of $f(\xi)$ as the fraction of a population then we want $f \geq 0$. This means that, for our present purpose, we discard the solutions with $c < 2$.

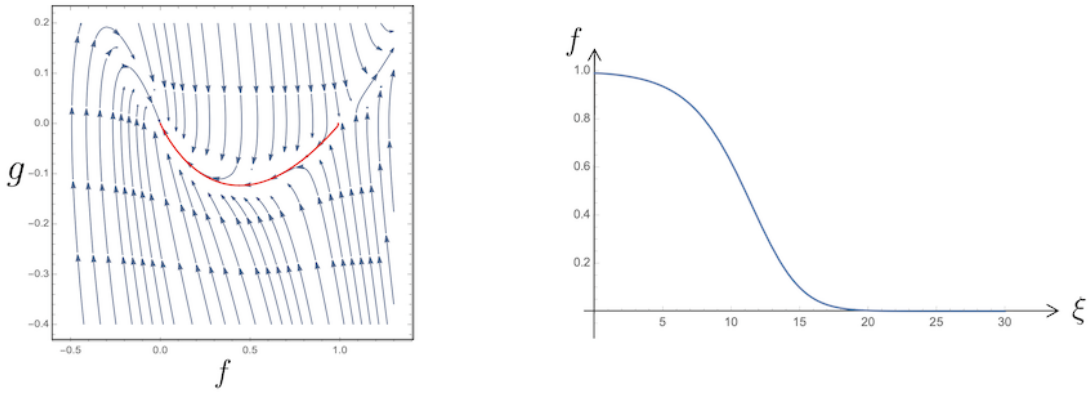


Figure 44. Numerical solutions with $c = 2$, both in the phase plane (on the left) and the evolution of $f(\xi)$. Again, the red line shows the trajectory of a solution that starts close to the unstable fixed point $(f, g) = (1, 0)$.

That leaves us with $c \geq 2$. Here there is no such concern. A numerical plot of this solution (shown with $c = 2$) is depicted in Figure 44. Now there is a solution that starts near the unstable fixed point and heads directly towards the stable fixed point. These are the class of solutions that we will be interested in.

It's worth pointing out that something a little strange has happened here. We wanted to find solutions where we start at $f = 0$ and then perturb slightly to see what happens. Instead, our phase space analysis has resulted in solutions that seem to go the opposite way, with

$$f(\xi) \to 1 \quad \text{and} \quad \xi \to -\infty \quad \text{and} \quad f(\xi) \to 0 \quad \text{as} \quad \xi \to +\infty \ . \tag{3.88}$$

In fact, this is just because the ξ coordinate is defined as $\xi = x - ct$ and that minus sign is the cause for the strange behaviour. For fixed x, these same solutions obey $f(t) \to 0$ as $t \to -\infty$ and $f(t) \to 1$ as $t \to +\infty$.

A Mechanical Analogy

There's a way to translate the story above into something familiar. The equation (3.84) is the kind of thing that we studied in our course on Dynamics and Relativity. If we write it as

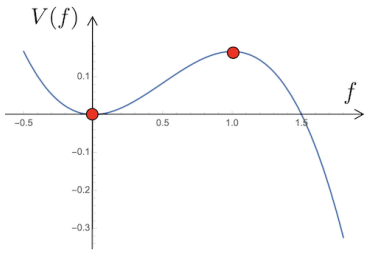
$$f'' = f(f-1) - cf' = -\frac{dV}{df} - cf' \tag{3.89}$$

with

$$V(f) = \frac{1}{2}f^2 - \frac{1}{3}f^3 \ . \tag{3.90}$$

then it looks like the equation of motion for a particle moving in potential V with a friction term $-cf'$.

The potential is plotted in the figure. It has two critical points, at $f = 0$ and at $f = 1$. In this analogy, as in the dynamical system, the point $f = 1$ is unstable and the point $f = 0$ is stable. That's compatible with what we saw above: in the $\xi = x - ct$ coordinate, we go flow from $f = 1$ to $f = 0$ rather than the other way around.



We've seen above that we get qualitatively different behaviour for $c < 2$ and for $c > 2$. It's simple to see why in this mechanical analogy, where c dictates the strength of the friction force. For $c < 2$, the system is "underdamped", meaning that, as it rolls down the hill, it overshoots the minimum at $f = 0$, oscillating back and forth before settling down. This is the behaviour seen in Figure 43.

In contrast, for $c > 2$ the system is overdamped, slowing enough so that it stops when it ultimately reaches the minimum at $f = 0$. The phase plane analysis tells us that the crossover between these two behaviours happens at $c = 2$ when the system has critical damping.

Linearised Analysis

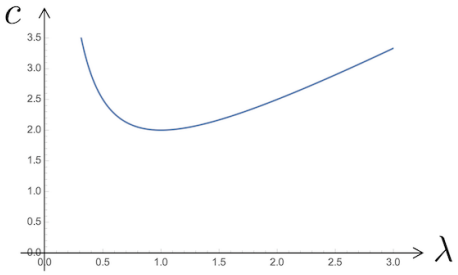
We can learn more about the travelling wave by looking at the leading edge of the wave, where $f \approx 0$. This means that we're looking at the region of the $f(\xi)$ graph in Figure 44 where $f(\xi)$ is approaching the ξ-axis. Here it's appropriate to linearise the equation (3.84) and work with

$$-cf' = f'' + f \ . \tag{3.91}$$

We make the obvious ansatz $f(\xi) = e^{-\lambda\xi}$, with $\lambda > 0$ so that this solution decays towards $f \to 0$ as ξ increases. We see that this solves the equation if

$$\lambda^2 - c\lambda + 1 = 0 \quad \Longrightarrow \quad c = \lambda + \frac{1}{\lambda} \ . \tag{3.92}$$

This is plotted in the figure. We can think of $1/\lambda$ as the width of the wavefront. We learn that the speed and shape of the wave are linked.



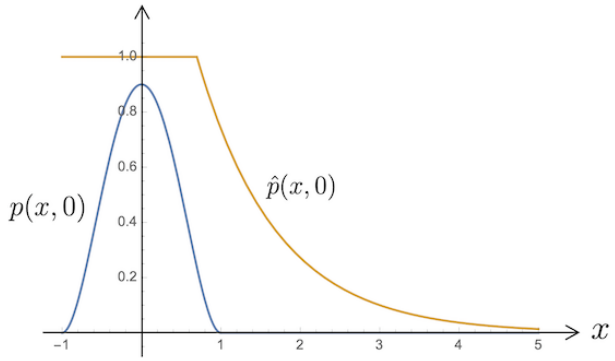


Figure 45. The initial profile $p(x,0)$ that evolves through the full non-linear equation is bounded above by the exponentially decaying profile $\hat{p}(x,0)$ that will evolve through the linearised Fisher equation.

The Speed of the Non-Linear Wave

So far, nothing has told us what speed c the wave travels at if we start with a given initial, localised perturbation $p(x,0)$. We only know that this speed must be $c \geq 2$.

The full non-linear analysis is complicated but the final result, proven by Kolomgorov, is beautifully simple. If we start with some initial conditions that vanish outside of some interval, i.e. $p(x,0) = 0$ for all $|x| > x_0$, the the system will ultimately settle down a wave that travels with speed $c = 2$. In other words, the non-linear system travels at the *slowest* possible speed of the linearised system.

We won't prove this result here, but we can motivate it with the following argument. First note that the non-linear speed must be *one* of the allowed linear speeds $c \geq 2$ just because the linearised analysis is valid at the wavefront. But, with suitably localised initial conditions, we can show that the non-linear speed must be less than (or equal to) that of a linear wave.

To see this, let's take initial conditions that are strictly localised in some region

$$p(x,0) = 0 \quad \text{for all } |x| \geq x_0 \ . \tag{3.93}$$

We'll evolve this with the full non-linear Fisher equation (3.82).

Our strategy is to set this profile in a race against a wavefront with initial profile

$$\hat{p}(x,0) = Ae^{-\lambda x} \ . \tag{3.94}$$

We will pick A so that $p(x,0) < \hat{p}(x,0)$. It's simple to check that this is always possible to construct such a bounding profile for any choice of $\lambda > 0$ simply by picking a suitable A. Crucially, we evolve the profile $\hat{p}(x,t)$ through the *linearised* Fisher equation

$$\frac{\partial \hat{p}}{\partial t} = \frac{\partial^2 \hat{p}}{\partial x^2} + \hat{p} \ . \tag{3.95}$$

Now we set these two profiles off. We will show that it's not possible for the non-linear $p(x,t)$ to overtake the linearised $\hat{p}(x,t)$. At heart, this follows because the missing term in the linearised equation is $-p^2$ and, with the minus sign, this only serves to delay the non-linear evolution.

We can put some meat on this argument by defining $g(x,t) = \hat{p}(x,t) - p(x,t)$. By construction, we have $g(x,0) > 0$. Watching this function evolve in time, we have

$$\frac{\partial g}{\partial t} = \frac{\partial \hat{p}}{\partial t} - \frac{\partial p}{\partial t} = \frac{\partial^2 g}{\partial x^2} + g + p^2 \geq \frac{\partial^2 g}{\partial x^2} + g \ . \tag{3.96}$$

We learn that the evolution of $g(x,t)$ is at least as fast as diffusion with linear growth. And with $g(x,0)$ positive, the function $g(x,t)$ can never go negative. This is telling us that $p(x,t)$ is bounded above by $\hat{p}(x,t)$ for all time. In other words, the non-linear wave can never overtake the linear wave.

But the analysis above holds for any choice of λ and, in particular, for $\lambda = 1$ which travels at the slowest speed $c = 2$. It tells us that the non-linear wave can travel no faster than $c = 2$. But, as we've seen previously, the wave ansatz only makes sense for $c \geq 2$. Hence the non-linear wave must travel at the slowest possible speed $c = 2$.

3.2.2 Front Propagation in Bistable Systems

Here is a simple modification of the Fisher equation

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial x^2} - p(p-r)(p-1) \ . \tag{3.97}$$

We'll take $0 < r < 1$.

Now, in the homogeneous system, both $p = 0$ and $p = 1$ are stable fixed points. The intermediate value of $p = r$ is unstable. For this reason, systems of this type are referred to as *bistable*.

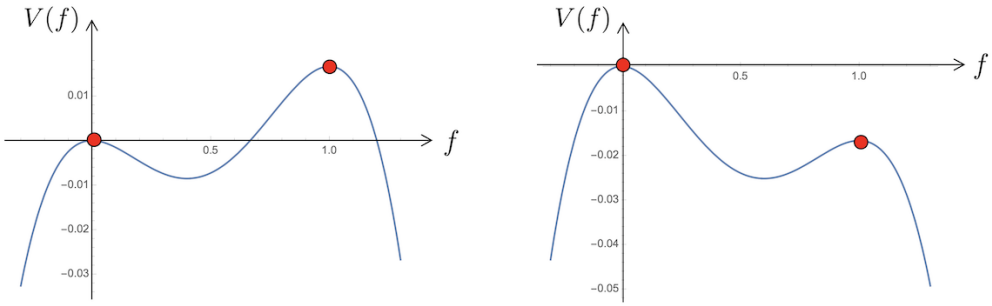
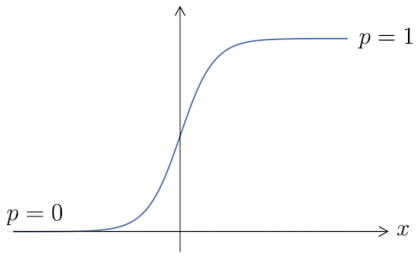


Figure 46. On the left: the potential $V(f)$ plotted with $r = 0.4$. On the right: the potential plotted with $r = 0.6$.



Suppose that we start in a system with $p = 0$ to the left, as $x \to -\infty$, and $p = 1$ to the right, as $x \to +\infty$. In between there has to be a transition, which we will call a "front". It looks something like the plot shown in the figure. The question that we would like to ask is: what happens next? Does the front advance to the left, or to the right? Since both $p = 0$ and $p = 1$ are stable fixed points, it's not immediately obvious which will win. We could think of this as a model for how diseases, mutations, or chemicals spread or die out.

We can use the kind of analysis that we developed for the Fisher equation to answer this. We will again look for a travelling wave solution, with

$$p(x,t) = f(\xi) \quad \text{with} \quad \xi = x - ct \tag{3.98}$$

for some velocity c. With this ansatz, the reaction-diffusion equation (3.97) becomes

$$-cf' = f'' - f(f-r)(f-1) \ . \tag{3.99}$$

This time we can get all the information we need from the mechanical analogy. We write

$$f'' = -\frac{dV}{df} - cf' \quad \text{with} \quad V(f) = -\frac{1}{4}f^4 + \frac{1}{3}(1+r)f^3 - \frac{1}{2}rf^2 \ . \tag{3.100}$$

This potential has two maxima, at $f = 0$ and $f = 1$. But, crucially, the shape of the potential depends on the value of r. For $r < 0.5$, the maximum at $f = 1$ is higher; for $r > 0.5$, the maximum at $f = 0$ is higher. Two representative examples are shown in Figure 46.

When $r < 0.5$, the ball rolls down from $f = 1$. If the friction term, captured by $-cf'$, is large, then the ball will ultimately come to rest at the local minimum at $f = r$. if the friction is low, then the ball will sail past the local maximum at $f = 0$ and into oblivion. In both cases, there is a formal solution to the reaction-diffusion equation but not one with the boundary conditions that we want. However, there is a special value of c such that the friction is just right and the ball rolls down from $f = 1$ where it sat at $\xi \to -\infty$, coming to rest at $f = 0$ at $\xi \to +\infty$. This is the velocity c that we want.

When $r > 0.5$, the heights of the two maxima are inverted, and now there is a critical velocity where the ball rolls the other way: from $f = 0$ to $f = 1$.

But, as in the previous section, we have to remember that the mechanical analogy reverses what actually happens because $\xi = x - ct$. This means that

- For $r < 0.5$ we have, for fixed x, $p(x,t) \to 1$ as $t \to \infty$ and so the front moves to the left.
- For $r > 0.5$ we have, for fixed x, $p(x,t) \to 0$ as $t \to \infty$ and so the front moves to the right.

In contrast to the Fisher equation, the mechanical analogy tells us that the front must travel at a very specific velocity c. But what is it? We can make progress by computing the analog of the work done in our mechanical system. We can take the equation of motion (3.100), multiply by f', and integrate. We have

$$\int_{-\infty}^{+\infty} d\xi \; f'f'' = \int_{-\infty}^{+\infty} d\xi \; \left(-f' \frac{dV}{df} - cf'^2 \right) = \int_{-\infty}^{+\infty} d\xi \; \left(-\frac{dV}{d\xi} - cf'^2 \right) \; . \quad (3.101)$$

The left-hand side is a total derivative of $\frac{1}{2}f'^2$ but our boundary conditions mean that $f' \to 0$ as $\xi \to \pm\infty$. This leaves us with an expression for the velocity

$$c = -\frac{\Delta V}{\int d\xi \; f'^2} \; . \quad (3.102)$$

Here ΔV is the difference in energy between the two maxima,

$$\Delta V = V(f = 1) - V(f = 0) = \frac{1}{6}\left(\frac{1}{2} - r \right) \; . \quad (3.103)$$

Note that if $r < 0.5$ then $\Delta V > 0$ and so $c < 0$ and the front travels to the left. Meanwhile, if $r < 0.5$ then $c > 0$ and the front travels to the right. This agrees with what we saw above.

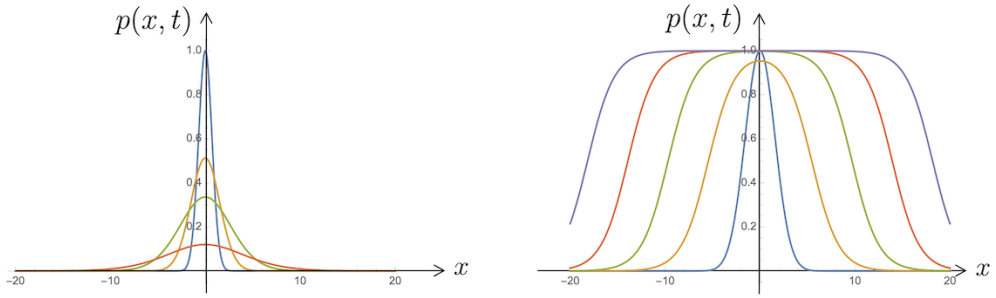


Figure 47. Numerical solutions for $r = 0.2$. The plot on the left starts with the initial condition $p(x, 0) = e^{-x^2}$. The one on the right starts with the wider initial condition $p(x, 0) = e^{-x^2/5}$. We see that the first flounders while the second flourishes.

To determine the actual speed c, we still need to do the integral $\int d\xi\ f'^2$. And, for this, we typically need to first figure out the solution $f(\xi)$. That's not so easy, but there is one value of r for which we can solve the equation of motion exactly. This is the value $r = 0.5$, when the local maxima of the potential have the same height and, correspondingly, the front is static with $c = 0$ and doesn't move. In this case, you can check that the function $f(\xi)$ is given by

$$f = \frac{1}{2}\left(1 - \tanh\left(\frac{\xi}{2\sqrt{2}}\right)\right) \ . \tag{3.104}$$

If we are cheeky and use this as a proxy for the function $f(\xi)$ in the integral, then we get a speed

$$c = 2\left(r - \frac{1}{2}\right) \ . \tag{3.105}$$

Strictly, this calculation holds only when $r = 0.5$ where the speed vanishes! But we can view this as a good approximation to the speed for $r \approx 0.5$. Indeed, if we were more careful we could set up a perturbation expansion in $r - 0.5$, with this the leading order term.

Localised Perturbations

There's a closely related question that we can ask of this system? Suppose that we start in the $p = 0$ state but then introduce a small region of $p = 1$ state, localised around the origin. What then happens? Does this $p = 1$ state expand to take over the world? Or does the $p = 0$ state fight back and shrink it?

The analysis that we've done above goes part way towards answering this. If $r > 0.5$ then the $p = 0$ state will win and the $p = 1$ insurgents will be crushed. Meanwhile, $r < 0.5$ then there's an opportunity for the $p = 1$ state to expand. But it's not guaranteed. That's because our previous analysis assumed that the system settled down to some wavelike behaviour with the fronts propagating at some constant speed. But the question of when this happens depends on how wide the initial localised perturbation is.

We won't give any detailed analysis of this behaviour here, but instead exhibit some simple numerical solutions. Figure 47 shows the time evolution of two different initial perturbations, the one on the left narrower than the one on the right. You can see clearly that the one on the left shrinks over time, while the one on the right thrives, ultimately forming wavefronts that are described by the analysis we did previously.

Dengue Revisited

We can connect the analysis above to one of the stories that we met earlier in these lectures. In Section 1.4.5, we described how Wolbachia bacteria could be introduced to mosquitos to inhibit the spread of dengue fever. Our model of choice was the two-dimensional dynamical system (1.137)

$$\frac{du}{dt} = u\left(u_0 - \frac{v}{u+v} - (u+v)\right) \quad \text{and} \quad \frac{dv}{dt} = v\left(v_0 - (u+v)\right) \ . \tag{3.106}$$

Here u is the population of uninfected mosquitoes and v the infected. The two constants are restricted to lie in $0 < v_0 < u_0 < 1$. (We've switched variables from x and y in (1.137) to u and v above to avoid confusion with the spatial coordinate x that we will soon introduce.)

This is a two-dimensional dynamical system, but it has hidden within it a one-dimensional system that governs the fraction of infected mosquitos

$$p = \frac{v}{u+v} \ . \tag{3.107}$$

You can check that the dynamics of p is governed by

$$\frac{dp}{dt} = -p(p-r)(p-1) \tag{3.108}$$

with $r = u_0 - v_0 \in (0, 1)$. This is precisely the homogeneous system that we discussed above. We can upgrade it to a system that includes spatial localisations by promoting $p(t)$ to a function $p(x, t)$. If we further assume that the population of infected mosquitos diffuses then we are back to solving the equation (3.97). We learn that a localised population of infected mosquitos will only spread if the parameter $r = x_0 - y_0 < 0.5$.

Admittedly this analysis also assumed, perhaps unrealistically, that the mosquitos fly only along a one-dimensional line. You might want to upgrade the system further to allow for 2d diffusion and redo the analysis before you contact the WHO.

Waves in Higher Dimensions

It's reasonably straightforward to extend the analysis above to waves in higher dimensions. Indeed, for plane waves, the story is identical. But for axially symmetric (in 2d) or spherically symmetric (in 3d) there's an additional term that we have to deal with. For example, a 2d axially symmetric system, the Fisher equation reads

$$\frac{\partial p}{\partial t} = \frac{\partial^2 p}{\partial r^2} + \frac{1}{r}\frac{\partial p}{\partial r} + p(1-p) \ . \tag{3.109}$$

Now we get that extra $\partial p/\partial r$ term on the right-hand side. For waves with $c > 0$, on the wavefront, $\partial p/\partial r < 0$. You can see this in the plots in Figure 47 so this additional term acts to slow the wave down. However, it also comes with a $1/r$ which means that it plays less of a role as the spreading circle gets big and the boundary looks more like a plane wave. The upshot is that the wave speed approaches $c \to 2$ as $r \to \infty$.

3.2.3 Wave Propagation in Neurons

We met a model for how neurons are excited in Section 1.7. Our slimmed-down model of choice was due to FitzHugh and Nagumo and was described by the following pair of ordinary differential equations (1.192)

$$\begin{aligned} \epsilon \frac{du}{dt} &= u + v - \frac{1}{3}u^3 \\ \frac{dv}{dt} &= -(u - a + bv) \ . \end{aligned} \tag{3.110}$$

Here $u(t)$ represents the voltage difference across a membrane, while $v(t)$ represents the ease with which various ions can cross the membrane. The constants a and b sit in the region

$$0 < b \leq 1 \ , \quad 1 - \frac{2b}{3} < a < 1 \ . \tag{3.111}$$

Meanwhile, we take $\epsilon \ll 1$ to ensure that the dynamics of $u(t)$ is fast, while that of $v(t)$ is much slower. This separation into two times scales is, in part, responsible for the interesting property of these equation: namely that a small stimulus gives rise to a large response which, in the context of neurons, is known as the action potential.

Now we extend (3.110) to include spatial propagation. First, we take both variables to depend on space and time, so we have $u(t,x)$ and $v(t,x)$. The voltage difference u diffuses, but v does not. Correspondingly, we extend the equations (3.110) to

$$\begin{aligned} \epsilon \frac{du}{dt} &= u + v - \frac{1}{3}u^3 + \epsilon^2 \frac{\partial^2 u}{\partial x^2} \\ \frac{dv}{dt} &= -(u - a + bv) \ . \end{aligned} \tag{3.112}$$

The diffusion term comes with a ϵ^2 to ensure that the spatial and temporal variations are both fast.

We will again search for travelling wave solutions of the form

$$u(x,t) = u(\xi) \quad \text{and} \quad v(x,t) = v(\xi) \quad \text{with} \quad \xi = x - ct \ . \tag{3.113}$$

Substituting this ansatz into the equations (3.112), we arrive at the pair of ordinary differential equations

$$\begin{aligned} -\epsilon c u' &= u + v - \frac{1}{3}u^3 + \epsilon^2 u'' \\ -cv' &= -(u + a + bv) \ . \end{aligned} \tag{3.114}$$

We could eliminate $v(\xi)$ from this pair of equations, but only at the expense of having a third order differential equation for $u(\xi)$. That makes the problem somewhat harder to solve than the analogous equation (3.84) for the Fisher equation.

To proceed, we're going to make use of the two different time scales in the problem, encapsulated in the small $\epsilon \ll 1$ factors in the equations. We know from our previous analysis that the spatially homogeneous system undergoes a cycle as shown in Figure 48 (which is a repeat of Figure 27). We split this cycle into four distinct pieces, labelled AB, BC, CD, and DA. (The beginning and final point are both labelled A even though they are slightly separated.) From the figure, we can see that the transitions AB and CD happed rapidly, while BC and DA are more leisurely. This gives us the motivation to look at each in turn.

Fast from A to B: For the fast motion, it is appropriate to rescale the spacetime coordinate and write

$$\xi = \epsilon\zeta \ . \tag{3.115}$$

With this rescaling, the equations (3.114) become

$$\begin{aligned} -cu' &= u + v - \frac{1}{3}u^3 + u'' \\ -cv' &= -\epsilon(u + a + bv) \end{aligned} \tag{3.116}$$

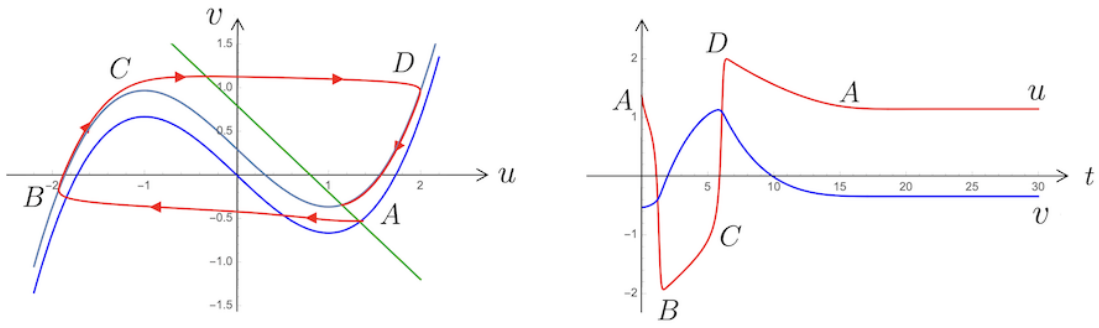


Figure 48. The phase plane motion (on the left, in red) and time dependence (on the right) for the spatially homogeneous model. These are now split into four distinct segments, labelled AB, BC, CD and DA.

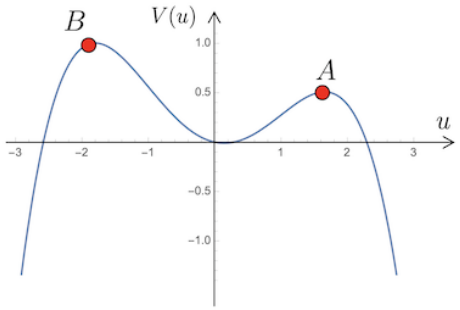
where the primes now denote differentiation with respect to ζ, rather than ξ. The $\epsilon \ll 1$ has now shifted to the right-hand side of the second equation, telling us that v is approximately constant, and equal to its fixed point value $v^\star$, on this segment. Indeed, this can also be seen in the plots of Figure 48 which confirms that the fixed point sits in the region $-1 < v^\star < 0$. This means that the dynamics is captured by the single, second order differential equation

$$-cu' = u + v^\star - \frac{1}{3}u^3 + u'' \ . \tag{3.117}$$

Now we're in business: this is the same kind of equation that we met previously and we have various ways to think about it. For example, if we embrace the mechanical analogy, we write

$$u'' = -\frac{dV}{d\zeta} - cu' \quad \text{with} \quad V(u) = -\frac{1}{12}u^4 + \frac{1}{2}u^2 + v^\star u. \tag{3.118}$$

The potential is plotted in the figure to the right. We see that this is the same kind of bistable system that we met in Section 3.2.2. In the mechanical analogy, the ball rolls down from the global maximum at B towards the local maximum at A. (Recall that things run from B to A, rather than A to B, in the mechanical analogy because our "time" is $\xi = x - ct$ with that minus sign in front of ct.) The is a critical value of the friction coefficient c for



which the ball miraculously ends up perched at the point A. This determines the speed c of the propagating wave. An expression for this critical velocity can be derived using (3.102).[10]

Slow from B to C: The next phase of the cycle, from B to C. For this, we should return to our original unscaled variable ξ and drop the terms proportional to $\epsilon \ll 1$ in (3.114). We're left with

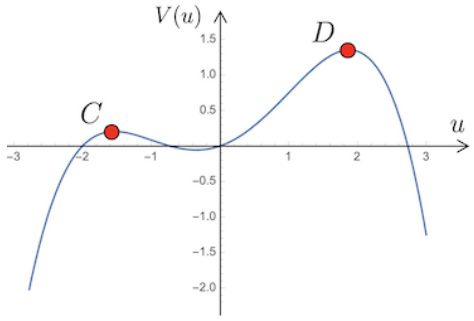
$$v = \frac{1}{3}u^3 - u \quad \text{and} \quad -cv' = -(u + a + bv) \ . \tag{3.119}$$

The first of these equations is telling us that the dynamics lies on the slow manifold, which is the cubic shown on the left of Figure 48. The second equation is just a first order system. We learn that the value of v slowly increases.

The question that we would like to ask is: at what value of v does the system exit this slow motion? Let's call this value $v^{\star\star}$. You might naively think that this is the same value of $v^{\star\star}$ that appears in the spatially homogeneous system shown in Figure 48. But that turns out *not* to be the case. To see why, we need to turn to the next phase of the cycle.

Fast from C to D: The transition from C to D is again fast and we can use the same analysis as we saw from A to B. We're again left with the equation (3.117), but now with the fixed point $v^\star$ replaced by the new value $v^{\star\star}$

$$-cu' = u + v^{\star\star} - \frac{1}{3}u^3 + u'' \ . \tag{3.120}$$



We will have $v^{\star\star} > 0$ (which contrasts with $v^\star < 0$. This ensures that the effective potential in (3.118) has the positions of the local and global maxima swapped, so that the dynamics goes the other way. An example of such a potential is shown on the right. But what is the value of $v^{\star\star}$?

At this point, we use a variant of our previous argument. In the mechanical analogy, we want to roll from point D to point C with a critical value of the "friction" c so

[10] You can watch an experiment measuring the velocity of these action potentials in earthworms in this Youtube video. (Be warned: it does involve sticking pins into an anesthetised earthworm, although the author of the video promised that the worm was then released back into the garden where it lived a long and rewarding life.)

that we end up perched precisely at the local maximum C. Usually we would use this argument to determine c. But, in the present case, we already know the value of c: it was determined by our analysis of the AB part of the cycle. So now we replay this argument, but now varying the value of $v^{\star\star}$, so that the effective potential changes until the two maxima are exactly the right height to allow a trajectory from D to C that works for the chosen value of c. In that we, we find the value of $v^{\star\star}$ that allows the entire pulse – from A to B to C to D to A again – to all propagate at the same speed c.

Slow from D to A: The final part of the story, from D to A, is again a gentle relaxation along the slow manifold. This is described by the pair of equations (3.119). This concludes the cycle. The end result is that all parts of the pulse propagate at the speed c that was determined by the $A \to B$ part of the analysis.

3.3 Turing Instability

As we have seen, diffusion encourages things to spread out, damping any wild spatial variations. This makes it rather surprising that, in the right circumstances, diffusion can render a system unstable giving rise to spatial variations. This is known as the Turing instability.

For this to occur, we need multiple variables. We'll consider the simplest such system with just two variables. $u(\mathbf{x}, t)$ and $v(\mathbf{x}, t)$, subject to the reaction-diffusion equations

$$\frac{\partial u}{\partial t} = f(u, v) + D_1 \nabla^2 u \quad \text{and} \quad \frac{\partial v}{\partial t} = g(u, v) + D_2 \nabla^2 v \ . \tag{3.121}$$

We have two diffusion constants, D_1 and D_2, and two functions $f(u, v)$ and $g(u, v)$ that determine the dynamics.

We will assume that, in the absence of diffusion, the dynamics admits a stable fixed point $(u^\star, v^\star)$ such that

$$f(u^\star, v^\star) = g(u^\star, v^\star) = 0 \ . \tag{3.122}$$

The Jacobian is

$$J = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{(u^\star, v^\star)} \tag{3.123}$$

where we're using the notation $f_u = \partial f / \partial u$ and so on. The statement that the fixed point is stable means that we have

$$\begin{aligned} \text{Tr}\, J &= f_u + g_v < 0 \\ \det J &= f_u g_v - f_v g_u > 0 \ . \end{aligned} \tag{3.124}$$

Now we consider perturbations that are not spatially homogeneous. We will write

$$u(\mathbf{x},t) = u^\star + \hat{u}(t)e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{and} \quad v(\mathbf{x},t) = v^\star + \hat{v}(t)e^{i\mathbf{k}\cdot\mathbf{x}} \ . \tag{3.125}$$

This notation deserves some explanation because suddenly, without warning, our variables $u(\mathbf{x},t)$ and $v(\mathbf{x},t)$ appear to be complex! This is just a trick. We will work with the form only when linearising about the fixed point, which means that we're always able to take real and imaginary parts at will. We could just as easily write $\cos(\mathbf{k}\cdot\mathbf{x})$ instead of $e^{i\mathbf{k}\cdot\mathbf{x}}$. We prefer the latter because it's typically easier to work with exponentials than trigonometric functions.

What happens with such a perturbation? If we substitute this ansatz into (3.121) and keep only terms linear in $\hat{u}$ and $\hat{v}$, then we get the equations

$$\begin{aligned} \frac{d\hat{u}}{dt} &= f_u\hat{u} + f_v\hat{v} - D_1k^2\hat{u} \\ \frac{d\hat{v}}{dt} &= g_u\hat{u} + g_v\hat{v} - D_2k^2\hat{v} \end{aligned} \tag{3.126}$$

with $k^2 = \mathbf{k}\cdot\mathbf{k}$ and where f_u and other partial derivatives are all evaluated at the fixed point.

Your first inclination is to think that the diffusion terms only make the system more stable. After all, they both appear with negative signs on the right-hand side! But that's not the way these things work! To check stability, we have to look at the modified Jacobian,

$$J_{\text{new}} = \begin{pmatrix} f_u - D_1k^2 & f_v \\ g_u & g_v - D_2k^2 \end{pmatrix} \ . \tag{3.127}$$

This has

$$\text{Tr}\, J_{\text{new}} = \text{Tr}\, J - (D_1 + D_2)k^2 < 0 \ . \tag{3.128}$$

So the trace is indeed more negative. This is what our previous intuition was telling us. However, the determinant is not so straightforward. It is

$$\begin{aligned} \det J_{\text{new}} &= (f_u - D_1k^2)(g_v - D_2k^2) - f_vg_u \\ &= \det J - k^2(D_1g_v + D_2f_u) + D_1D_2k^4 \ . \end{aligned} \tag{3.129}$$

The system is stable only if $\det J_{\text{new}} > 0$. But we see that this is not guaranteed! There's that middle term which could possibly turn the whole thing negative.

To see if this happens, we write

$$\det J_{\rm new} = Ak^4 - Bk^2 + C \ . \tag{3.130}$$

This dips below zero for some region of $k^2 > 0$ only if $B > 0$ and the quadratic has real roots. This, in turn, requires that the discriminant $B^2 - 4AC$ is positive. Translated back to the expression (3.129), we learn that the determinant can be negative for certain values of k provided that

$$D_1 g_v + D_2 f_u > \sqrt{4D_1 D_2 (f_u g_v - f_v g_u)} \ . \tag{3.131}$$

This is the condition for *Turing Instability*.

Note that the system is stable to both long wavelength modes (with $k \ll 1$) and short wavelength modes (with $k \gg 1$). The long wavelength modes are close to the homogeneous system which is known to be stable. The short wavelength modes are eliminated quickly by diffusion. The instability occurs only in some intermediate regime,

$$k_\star^2 - \Delta < k^2 < k_\star^2 + \Delta \tag{3.132}$$

with

$$k_\star = \sqrt{\frac{B}{2A}} \quad \text{and} \quad \Delta = \frac{\sqrt{B^2 - 4AC}}{2A} \ . \tag{3.133}$$

You could imagine starting with a system that does not exhibit the Turing instability, and then slowly varying parameters until you reach the phase transition at $B^2 = 4AC$. At this point, the modes with wavenumber

$$k_\star = \left(\frac{C}{A}\right)^{1/4} = \left(\frac{\det J}{D_1 D_2}\right)^{1/4} \tag{3.134}$$

are the first to become unstable.

Instability Requires Different Diffusivities

The Turing instability feels counterintuitive. At heart, the idea is that the matrix J has eigenvalues with negative real parts, but the matrix

$$J_{\rm new} = J - k^2 \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix} \tag{3.135}$$

does not. It feels like subtracting things off the diagonal should only decrease both eigenvalues. But, as we have seen, it's possible to decrease one and increase the other. That's the algebraic crutch on which the instability relies

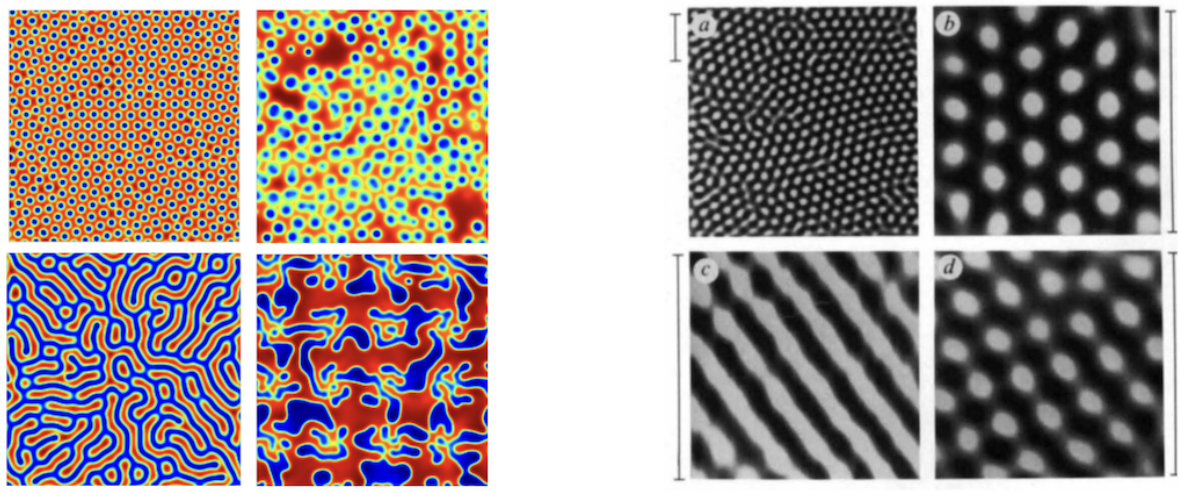


Figure 49. On the left: numerical simulations of various reaction-diffusion systems with a Turing instability. On the right: Turing instabilities seen in chemical reactions.

For this to happen, however, it's important that $D_1 \neq D_2$. Indeed, if $D_1 = D_2 = D$ then we have $J_{\rm new} = J - k^2 D\mathbb{1}$. If the eigenvalues of J are λ_i then the eigenvalues of $J_{\rm new}$ are $\lambda_i - k^2 D$ and both decrease.

Another way of seeing this is to define the ratio of diffusivities

$$d = \frac{D_1}{D_2} \ . \tag{3.136}$$

Then the condition for instability (3.131) becomes

$$f_u + dg_v > 2\sqrt{d \det J} \ . \tag{3.137}$$

The right-hand side is clearly greater than zero so we must have

$$f_u + dg_v > 0 \ . \tag{3.138}$$

Meanwhile, we know that

$$\mathrm{Tr}\, J = f_u + g_v < 0 \ . \tag{3.139}$$

So clearly $d = 1$ does not do the job. For an instability to kick, the diffusivities must be suitably different. Moreover, this simple algebra highlights what's actually going on. For the instability to occur, one of f_u and g_v must be positive and the other negative. Suppose that we have $f_u > 0$ and $g_v < 0$. Then the variable u is called an *activator*

Figure 50. This is Eddie, possibly Turing unstable, definitely not Turing complete.

because it wants to increase things while the variable v is called the *inhibitor* because it wants to reduce things. The result (3.139) is telling us that, in the homogeneous situation, the inhibitor wins. But if we take $d \ll 1$, so the inhibitor diffuses faster than the activator, then the result (3.137) is telling us that, ultimately the activator can triumph.

3.3.1 Pattern Formation

Our analysis above only finds the instability. Obviously the next question is: what becomes of it? We know that the system will necessarily become inhomogeneous and we might expect that this happens at a characteristic wavelength

$$\lambda_\star \approx \frac{2\pi}{k_\star} \tag{3.140}$$

To understand the resulting pattern, we need to study the full non-linear behaviour of a system. And this typically means doing numerics. Some examples of patterns from various numerical simulations, together with experimental results seen in certain chemical reactions are shown in Figure 49.[11]

It is thought that other pattens seen in nature, including animals coats, can be traced to a Turing diffusion instability of the kind described above.

[11]The numerical plots are taken from this blogpost which includes the script used to create them. The experimental data is taken from the paper Transition from a uniform state to hexagonal and striped Turing patterns, by Q. Ouyang and H. Swinney, Nature, 1991.

Effects of a Boundary

In the above discussion, we took our perturbations (3.125) proportional to $e^{i\mathbf{k}\cdot\mathbf{x}}$. This is appropriate for an infinite domain. But it may be that we want to solve the reaction-diffusion equation on some finite domain. Typically we would then impose Neumann boundary conditions $\mathbf{n}\cdot\nabla u = \mathbf{n}\cdot\nabla v = 0$ on the boundary ∂V, where $\mathbf{n}$ is the vector normal to the boundary. We should now take the perturbations to be eigenfunctions of the Laplacian on this domain, rather than $e^{i\mathbf{k}\cdot\mathbf{x}}$.

In a finite domain, the eigenvalues k^2 will typically be discrete and we get an instability if one of them lies in the window (3.132). The lowest eigenvalue k_0 is set by the size L of the domain,

$$k_0 \approx \frac{2\pi}{L} \ . \tag{3.141}$$

If the system is suitably small, the we will have $k_0^2 > k_\star^2 + \Delta$ and no instability will occur. This mimics what we saw in Section 3.1.3, where linear growth does not lead to an instability for small system sizes.

Suppose, for example, that the domain consists of a rectangle with $x \in [0, L_1]$ and $y \in [0, L_2]$. Then the eigenvalues of the Laplacian are $e^{i\mathbf{k}\cdot\mathbf{x}}$ but with $\mathbf{k}$ quantised as

$$k_1 = \frac{m\pi}{L_1} \quad \text{and} \quad k_2 = \frac{n\pi}{L_2} \quad m, n \in \mathbb{Z} \ . \tag{3.142}$$

If the rectangle is reasonably large and square, then one would expect to find k_1 and k_2 sitting within the window of instability (3.132). As we've stressed, it's far from clear what the resulting pattern would be but suppose that we end up with spots. Now consider a narrower rectangle, say with $L_2 \ll L_1$. Then we could have a situation in which there is no instability in the y-direction, but only in the x-direction, resulting in stripes rather than spots. This suggests that if the Turing instability is responsible for animal patterns then we might expect to see animals with spotted coats, but striped tails.

3.3.2 An Example

Our discussion above was rather abstract. It's useful to have one example where we can see this in practice. We take

$$\frac{\partial u}{\partial t} = -u + u^2 v + \nabla^2 u \quad \text{and} \quad \frac{\partial v}{\partial t} = b - u^2 v + d\nabla^2 v \ . \tag{3.143}$$

The model depends on just two parameters, b and the ratio of diffusivities d. You can think of this as modelling a chemical reaction, with two molecules u and v combining

as $2u + v \to 3u$. In addition, the u molecule decays at a constant rate (hence the $-u$ term) and the v molecule is produced at a constant rate (the $+b$ term). This is variant of the so-called Gray-Scott model.

First we look at the homogeneous situation. There is a single fixed point $(u^\star, v^\star) = (b, 1/b)$ with Jacobian

$$J = \begin{pmatrix} -1 + 2u^\star v^\star & u^{\star\,2} \\ -2u^\star v^\star & -u^{\star\,2} \end{pmatrix} = \begin{pmatrix} 1 & b^2 \\ -2 & -b^2 \end{pmatrix} \ . \tag{3.144}$$

We have $\mathrm{Tr}\, J = 1 - b^2$. And we have $\det J = b^2 > 0$. So the fixed point is stable for $b > 1$.

Now we include the diffusion term. Our modified Jacobian becomes

$$J_{\rm new} = \begin{pmatrix} 1 - k^2 & b^2 \\ -2 & -b^2 - dk^2 \end{pmatrix} \ . \tag{3.145}$$

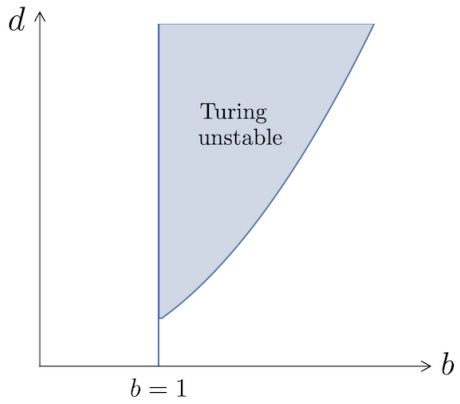
The determinant is

$$\det J_{\rm new} = dk^4 - (d - b^2)k^2 + b^2 \ . \tag{3.146}$$

We require $d > b^2 > 1$ for the roots to be positive. Indeed, we knew from our general discussion that $d = 1$ wouldn't do the job because the diffusivities had to be different. This quadratic (in k^2) has roots provided that

$$d - b^2 \geq 2b\sqrt{d} \ . \tag{3.147}$$

A little bit of algebra shows that this holds provided $d > (3 + 2\sqrt{2})b^2$ (using the fact that $b > 1$). The region of parameter space that exhibits the Turing instability is shown in the figure.



3.4 Chemotaxis

Bacteria and other single-celled organisms may be small, but they know what they like. They will happily swim towards nutrients, or away from poison, following the gradients of the chemical. This process is known as *chemotaxis*.

We will model the situation with two variables: $n(\mathbf{x}, t)$ is the density of bacteria and $c(\mathbf{x}, t)$ is the density of some chemical that they have developed a fondness for. For the chemical, we will have the usual kind of reaction-diffusion equation

$$\frac{\partial c}{\partial t} - D_c \nabla^2 c = G(n, c) \tag{3.148}$$

where $G(n, c)$ is some function that specifies the dynamics. However, for the bacteria we will include an additional term in the equation that captures the fact they swim towards the chemical. We have the general form

$$\frac{\partial n}{\partial t} + \nabla \cdot \mathbf{J} = F(n, c) \tag{3.149}$$

where $F(n, c)$ is a function that we will specify shortly, while the current is given by the now-familiar diffusion term, plus something else:

$$\mathbf{J} = -D_n \nabla n + n\mathbf{v} \ . \tag{3.150}$$

Here $\mathbf{v}$ is the velocity of the bacteria. They swim in the direction in which the chemical concentration is greatest, so we take

$$\mathbf{v} = \chi \nabla c \tag{3.151}$$

with $\chi > 0$ a constant.

Although the mathematical expression (3.151) is natural to write down, it's worth pausing to ask how it comes about physically. After all, bacteria are around 10^{-6} m long. It seems unlikely that they come equipped with sensitive equipment to allow them to detect the gradient of chemicals across such a small distance and then swim towards the place it's greatest! So what's the physics that leads to (3.151)?

The answer is pretty cool. Single-celled organisms with flagella have two modes of transport, called "runs" and "tumbling". On a run, they point themselves in one direction and motor along at a speed of around 10 - 50 μm per second. But every second or so, they stop and do a tumble, reorienting themselves in a random direction, before they head off again. The net effect is a random walk. The way they swim in the direction of greater chemical concentration is by reducing the frequency of tumbling when the concentration is higher, ensuring that they spend a longer time where the climate is nice.

The upshot is that our set of chemotaxis equations read

$$\begin{aligned}\frac{\partial n}{\partial t} &= D_n\nabla^2 n - \chi\nabla\cdot(n\nabla c) + F(n,c)\\ \frac{\partial c}{\partial t} &= D_c\nabla^2 c + G(n,c)\ .\end{aligned} \tag{3.152}$$

The novelty is, of course, the chemotaxis term proportional to χ. Our goal is to understand what qualitative effect this has on the dynamics., We will see that it provides another avenue for the system to become unstable.

3.4.1 An Example

We will explore the chemotaxis equations by looking at an example. We take

$$F(n,c) = \gamma - \delta n \quad \text{and} \quad G(n,c) = \alpha n - \beta c \tag{3.153}$$

with $\alpha, \beta, \gamma, \delta > 0$. The idea here is the bacteria are being constantly injected into the system, and then die at some rate δ. Meanwhile the bacteria are extreting their favourite chemical at a rate α, which is subsequently decaying at a rate β.

To start, we again assume that the system is homogenous and look for a fixed point $(n^\star, c^\star)$ of the local dynamics such that $F(n^\star, c^\star) = G(n^\star, c^\star) = 0$. There's a unique fixed point

$$(n^\star, c^\star) = \left(\frac{\gamma}{\delta}, \frac{\alpha\gamma}{\beta\delta}\right)\ . \tag{3.154}$$

The Jacobian at this fixed point is

$$J = \begin{pmatrix} -\delta & 0 \\ \alpha & -\beta \end{pmatrix}\ . \tag{3.155}$$

We see immediately that the two eigenvalues are $-\delta$ and $-\beta$ and both are negative. So our fixed point is stable.

Now we look at the effect of the gradient terms and, in particular, the chemotaxis term. We will perturb about the fixed point but, as in the previous section, allow our perturbations to vary in both space and time. We write

$$n(\mathbf{x},t) = n^\star + u(t)e^{i\mathbf{k}\cdot\mathbf{x}} \quad \text{and} \quad c(\mathbf{x},t) = c^\star + v(t)e^{i\mathbf{k}\cdot\mathbf{x}}\ . \tag{3.156}$$

We take both $u(t)$ and $v(t)$ to be small which means that, when substituting into the chemotaxis equations (3.152), we drop all terms quadratic or higher in these variables. We're then left with the following pair of equations

$$\begin{aligned}\frac{\partial u}{\partial t} &= -D_n k^2 u + \chi n^\star k^2 v - \delta u \\ \frac{\partial v}{\partial t} &= -D_c k^2 + \alpha u - \beta v \ .\end{aligned} \tag{3.157}$$

Now we have a slightly different dynamical system, with a modified Jacobian matrix

$$J_{\rm new} = J - k^2 \begin{pmatrix} D_n & -\chi\gamma/\delta \\ 0 & D_c \end{pmatrix} \ . \tag{3.158}$$

If the system is to be stable against spatially varying perturbations, then this new Jacobian $J_{\rm new}$ must also have negative eigenvalues. But does it?

First note that, in the absence of chemotaxis, with $\chi = 0$, the eigenvalues are again negative. So this system does not exhibit a Turing instability. But what happens when $\chi \neq 0$?

To compute the eigenvalues, we can look at

$$\mathrm{Tr}\, J_{\rm new} = -(\alpha+\beta) - k^2(D_n + D_c) < 0 \ . \tag{3.159}$$

So there's certainly no problem there. But the determinant gives

$$\det J_{\rm new} = (\alpha + k^2 D_n)(\alpha + k^2 D_c) - \frac{\alpha\gamma\chi}{\delta} k^2 \ . \tag{3.160}$$

The system is only stable if $\det J_{\rm new} > 0$. But we see that the chemotaxis term contributes with a minus sign. If you make χ big enough, then there is guaranteed to a window of k values for which the system goes unstable. Indeed, the mode with wavenumber k is unstable if

$$\frac{\alpha\gamma\chi}{\beta} > \frac{(\alpha + k^2 D_n)(\alpha + k^2 D_c)}{k^2} \ . \tag{3.161}$$

If we start with χ small and then slowly increase it, the first mode to go unstable is $k_\star$ which is the minimum of the function on the right-hand side above. A short calculation shows that this is given by

$$k_\star = \left(\frac{\beta\delta}{D_n D_c}\right)^{1/4} \ . \tag{3.162}$$

If we substitute this into (3.161), we find that the minimum value before the instability kicks in is

$$\chi_{\min} = \frac{\delta}{\alpha\beta}\left(\sqrt{\delta D_c} + \sqrt{\beta D_n}\right)^2 \ . \tag{3.163}$$

For $\chi > \chi_{\min}$, the system will again settle down to some spatially inhomogeneous configuration.