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Chapter 6

Front Propagation

6.1 Reaction-Diffusion Systems

We've studied simple $N = 1$ dynamical systems of the form

$$\frac{du}{dt} = R(u) \quad . \quad (6.1)$$

Recall that the dynamics evolves $u(t)$ monotonically toward the first stable fixed point encountered. Now let's extend the function $u(t)$ to the spatial domain as well, *i.e.* $u(\mathbf{x}, t)$, and add a diffusion term:

$$\frac{\partial u}{\partial t} = D \nabla^2 u + R(u) \quad , \quad (6.2)$$

where D is the diffusion constant. This is an example of a *reaction-diffusion system*. If we extend $u(\mathbf{x}, t)$ to a multicomponent field $\mathbf{u}(\mathbf{x}, t)$, we obtain the general reaction-diffusion equation (RDE)

$$\frac{\partial u_i}{\partial t} = D_{ij} \nabla^2 u_j + R_i(u_1, \dots, u_N) \quad . \quad (6.3)$$

Here, \mathbf{u} is interpreted as a *vector of reactants*, $\mathbf{R}(\mathbf{u})$ describes the *nonlinear local reaction kinetics*, and D_{ij} is the *diffusivity matrix*. If diffusion is negligible, this PDE reduces to decoupled local ODEs of the form $\dot{\mathbf{u}} = \mathbf{R}(\mathbf{u})$, which is to say a dynamical system at each point in space. Thus, any fixed point \mathbf{u}^* of the local reaction dynamics also describes a spatially homogeneous, time-independent solution to the RDE. These solutions may be characterized as dynamically stable or unstable, depending on the eigenspectrum of the Jacobian matrix $M_{ij} = \partial_i R_j(\mathbf{u}^*)$. At a stable fixed point, $\text{Re}(\lambda_i) < 0$ for all eigenvalues.

6.1.1 Single component systems

We first consider the single component system,

$$\frac{\partial u}{\partial t} = D \nabla^2 u + R(u) \quad . \quad (6.4)$$

Note that the right hand side can be expressed as the functional derivative of a *Lyapunov functional*,

$$L[u] = \int d^d x \left[\frac{1}{2} D(\nabla u)^2 - U(u) \right] , \quad (6.5)$$

where

$$U(u) = \int_0^u du' R(u') . \quad (6.6)$$

(The lower limit in the above equation is arbitrary.) Thus, eqn. 6.4 is equivalent to

$$\frac{\partial u}{\partial t} = - \frac{\delta L}{\delta u(\mathbf{x}, t)} . \quad (6.7)$$

Thus, the Lyapunov functional runs strictly downhill, *i.e.* $\dot{L} < 0$, except where $u(\mathbf{x}, t)$ solves the RDE, at which point $\dot{L} = 0$.

6.1.2 Propagating front solutions

Suppose the dynamical system $\dot{u} = R(u)$ has two or more fixed points. Each such fixed point represents a static, homogeneous solution to the RDE. We now seek a dynamical, inhomogeneous solution to the RDE in the form of a *propagating front*, described by

$$u(x, t) = u(x - Vt) , \quad (6.8)$$

where V is the (as yet unknown) front propagation speed. With this *Ansatz*, the PDE of eqn. 6.4 is converted to an ODE,

$$D \frac{d^2 u}{d\xi^2} + V \frac{du}{d\xi} + R(u) = 0 , \quad (6.9)$$

where $\xi = x - Vt$. With $R(u) \equiv U'(u)$ as in eqn. 6.6, we have the following convenient interpretation. If we substitute $u \rightarrow q$, $\xi \rightarrow s$, $D \rightarrow m$, and $v \rightarrow \gamma$, this equation describes the damped motion of a massive particle under friction: $m\ddot{q} + \gamma\dot{q} = -U'(q)$, where $\dot{q} = dq/ds$. The fixed points q^* satisfy $U'(q^*) = 0$ and are hence local extrema of $U(q)$. The propagating front solution we seek therefore resembles the motion of a massive particle rolling between extrema of the potential $U(q)$. Note that the stable fixed points of the local reaction kinetics have $R'(q) = U''(q) < 0$, corresponding to *unstable* mechanical equilibria. Conversely, unstable fixed points of the local reaction kinetics have $R'(q) = U''(q) > 0$, corresponding to *stable* mechanical equilibria. Note that

$$\mathcal{E} \equiv \frac{1}{2} D u_\xi^2 + U(u) \quad \Rightarrow \quad \frac{d\mathcal{E}}{d\xi} = -V u_\xi^2 \quad (6.10)$$

and thus $\mathcal{E}_\xi \leq 0$ if $V > 0$ while $\mathcal{E}_\xi > 0$ if $V < 0$.

Eqn. 6.9 is an $N = 2$ dynamical system of the form

$$\frac{d}{d\xi} \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} v \\ -D^{-1}R(u) - D^{-1}Vv \end{pmatrix} , \quad (6.11)$$

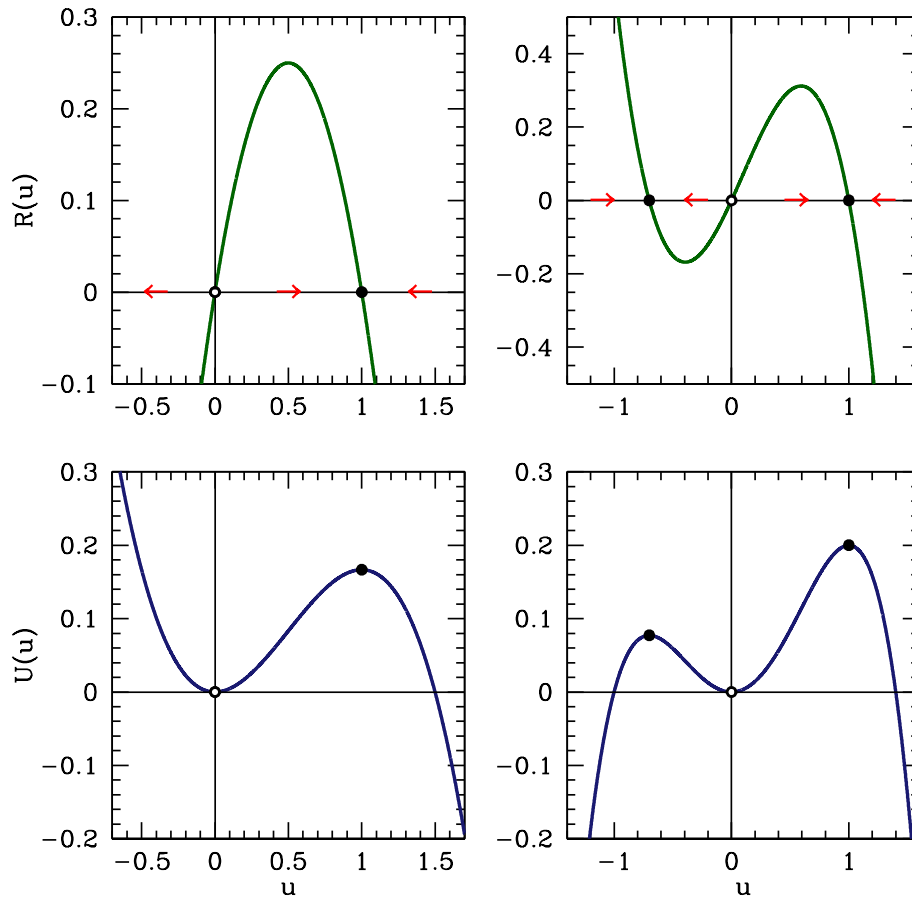


Figure 6.1: Reaction functions $R(u) = ru(a - u)$ with $r = a = 1$ (top left) and $R(u) = -ru(u - a)(u - b)$ with $r = 1$, $a = 1$, $b = -0.7$ (top right), along with corresponding potentials $U(u)$ (bottom panels). Stable fixed points for the local reaction kinetics are shown with a solid black dot, and unstable fixed points as a hollow black dot. Note that $R(u) = U'(u)$, so stable fixed points for the local reaction kinetics have $R'(u) = U''(u) < 0$, and thus correspond to *unstable* mechanical equilibria in the potential $U(u)$. Similarly, unstable fixed points for the local reaction kinetics correspond to *stable* mechanical equilibria.

with $v \equiv u'(\xi)$. At a fixed point (u^*, v^*) we must have $R(u^*) = 0$ and $v^* = 0$. The linearized dynamics at a fixed point are given by

$$\frac{d}{d\xi} \begin{pmatrix} \delta u \\ \delta v \end{pmatrix} = \overbrace{\begin{pmatrix} 0 & 1 \\ -D^{-1}R'(u^*) & -D^{-1}V \end{pmatrix}}^{M(u^*)} \begin{pmatrix} \delta u \\ \delta v \end{pmatrix} \quad (6.12)$$

We thus have

$$\tau(u^*) \equiv \text{Tr } M(u^*) = -D^{-1}V \quad , \quad \Delta(u^*) \equiv \det M(u^*) = D^{-1}R'(u^*) \quad . \quad (6.13)$$

Thus, if $R'(u^*) < 0$ the fixed point is a saddle, whereas if $R'(u^*) > 0$ the fixed point is stable if $V > 0$ and unstable if $V < 0$, and is a node if $R'(u^*) < V^2/4D$ and a spiral if $R'(u^*) > V^2/4D$.

A front solution corresponds to a mechanical motion interpolating between two equilibria at $u(\xi = \pm\infty)$. If the front propagates to the right then $V > 0$, corresponding to a positive (*i.e.* usual) friction coefficient γ . Any solution, therefore must start from an unstable equilibrium point u_1^* and end at another equilibrium u_{II}^* . The final state, however, may be either a stable or an unstable equilibrium for the potential $U(u)$. Consider the functions $R(u)$ and $U(u)$ in the left panels of fig. 6.1. Starting at 'time' $\xi = -\infty$ with $u = u_1^* = 1$, a particle with positive friction rolls down hill and eventually settles at position $u_{II}^* = 0$. If the motion is underdamped, it will oscillate as it approaches its final value, but there will be a solution connecting the two fixed points for an entire range of V values. Consider a model where

$$\begin{aligned} R(u) &= ru(u-a)(b-u) \\ U(u) &= -\frac{r}{4}u^4 + \frac{r}{3}(a+b)u^3 - \frac{r}{2}abu^2 \quad , \end{aligned} \quad (6.14)$$

with $a > 0 > b$, which is depicted in the right panels of fig. 6.1. Assuming $r > 0$, there are two stable fixed points for the local reaction kinetics: $u^* = a$ and $u^* = b$. Since $U(a) - U(b) = \frac{1}{12}r(a-b)^2(a^2 - b^2)$, the fixed point which is farther from $u = 0$ has the higher value. Without loss of generality, let us assume $|a| > |b|$, as is the case in the figure. One can then roll off the peak at $u^* = a$ and eventually settle in at the local minimum $u^* = 0$ for a range of V values, provided V is sufficiently large that the motion does not take u beyond the other fixed point at $u^* = b$. If we start at $u^* = b$, then a solution interpolating between this value and $u^* = 0$ exists for any positive value of V . As we shall see, this makes the issue of velocity selection a subtle one, as at this stage it appears a continuous family of propagating front solutions are possible. At any rate, for this type of front we have $u(\xi = -\infty) = u_1^*$ and $u(\xi = +\infty) = u_{II}^*$, where $u_{I,II}^*$ correspond to stable and unstable fixed points of the local dynamics. If we fix x and examine what happens as a function of t , we have $\xi \rightarrow \mp\infty$ as $t \rightarrow \pm\infty$, since $V > 0$, meaning that we start out in the unstable fixed point and eventually as the front passes over our position we transition to the stable fixed point. Accordingly, this type of front describes a *propagation into an unstable phase*. Note that for $V < 0$, corresponding to left-moving fronts, we have negative friction, meaning we move uphill in the potential $U(u)$. Thus, we start at $\xi = -\infty$ with $u(-\infty) = 0$ and end up at $u(+\infty) = u_{I,II}^*$. But now we have $\xi \rightarrow \pm\infty$ as $t \rightarrow \pm\infty$, hence once again *the stable phase invades the unstable phase*.

Another possibility is that one stable phase invades another. For the potential in the lower right panel of fig. 6.1, this means starting at the leftmost fixed point where $u(-\infty) = a$ and, with $V > 0$ and positive friction, rolling down hill past $u = 0$, then back up the other side, asymptotically coming to a perfect stop at $u(+\infty) = b$. Clearly this requires that V be finely tuned to a specific value so that the system dissipates an energy exactly equal to $U(a) - U(b)$ to friction during its motion. If $V < 0$ we have the time reverse of this motion. The fact that V is finely tuned to a specific value in order to have a solution means that we have a *velocity selection* taking place. Thus, if $R(a) = R(b) = 0$, then defining

$$\Delta U = \int_a^b du R(u) = U(b) - U(a) \quad , \quad (6.15)$$

we have that $u^* = a$ invades $u^* = b$ if $\Delta U > 0$, and $u^* = b$ invades $u^* = a$ if $\Delta U < 0$. The front velocity in either case is fixed by the selection criterion that we asymptotically approach both local maxima of $U(u)$ as $t \rightarrow \pm\infty$.

For the equation

$$Du'' + Vu' = ru(u-a)(u-b) \quad , \quad (6.16)$$

we can find an exact solution of the form

$$u(\xi) = \left(\frac{a+b}{2}\right) + \left(\frac{b-a}{2}\right) \tanh(A\xi) \quad . \quad (6.17)$$

Direct substitution shows this is a solution when

$$\begin{aligned} A &= |a-b| \left(\frac{r}{8D}\right)^{1/2} \\ V &= \sqrt{\frac{Dr}{2}} (a+b). \end{aligned} \quad (6.18)$$

6.1.3 Stability and zero mode

We assume a propagating front solution $u(x - Vt)$ connecting $u(-\infty) = u_L$ and $u(+\infty) = u_R$. For $|\xi|$ very large, we can linearize about the fixed points $u_{L,R}$. For $\xi \rightarrow -\infty$ we write $R(u_L + \delta u) \approx R'(u_L) \delta u$ and the linearized front equation is

$$D \delta u'' + V \delta u' + R'(u_L) \delta u = 0 \quad . \quad (6.19)$$

This equation possesses solutions of the form $\delta u = A e^{\kappa_L \xi}$, where

$$D \kappa_L^2 + V \kappa_L + R'(u_L) = 0 \quad . \quad (6.20)$$

The solutions are

$$\kappa_L = -\frac{V}{2D} \pm \sqrt{\left(\frac{V}{2D}\right)^2 - \frac{R'(u_L)}{D}} \quad . \quad (6.21)$$

We assume that u_L is a stable fixed point of the local dynamics, which means $R'(u_L) < 0$. Thus, $\kappa_{L,-} < 0 < \kappa_{L,+}$, and the allowed solution, which does not blow up as $\xi \rightarrow -\infty$ is to take $\kappa_L = \kappa_{L,+}$. If we choose $\xi_L < 0$ such that $\kappa_{L,+} \xi_L \ll -1$, then we can take as initial conditions $u(\xi_L) = u_L + A_L e^{\kappa_L \xi_L}$ and $u'(\xi_L) = \kappa_L A_L e^{\kappa_L \xi_L}$. We can then integrate forward to $\xi = +\infty$ where $u'(+\infty) = 0$ using the 'shooting method' to fix the propagation speed V .

For $\xi \rightarrow +\infty$, we again linearize, writing $u = u_R + \delta u$ and obtaining

$$D \delta u'' + V \delta u' + R'(u_R) \delta u = 0 \quad . \quad (6.22)$$

We find

$$\kappa_R = -\frac{V}{2D} \pm \sqrt{\left(\frac{V}{2D}\right)^2 - \frac{R'(u_R)}{D}} \quad . \quad (6.23)$$

If we are invading another stable (or metastable) phase, then $R'(u_R) < 0$ and we must choose $\kappa_R = \kappa_{R,-}$ in order for the solution not to blow up as $\xi \rightarrow +\infty$. If we are invading an unstable phase, however, then $R'(u_R) > 0$ and there are two possible solutions, with $\kappa_{R,-} < \kappa_{R,+} < 0$. In the $\xi \rightarrow \infty$ limit, the $\kappa_{R,+}$ mode dominates, hence asymptotically we have $\kappa_R = \kappa_{R,+}$, however in general both solutions are present asymptotically, which means the corresponding boundary value problem is underdetermined.

Next we investigate stability of the front solution. To do this, we must return to our original reaction-diffusion PDE and linearize, writing

$$u(x, t) = u(x - Vt) + \delta u(x, t) \quad , \quad (6.24)$$

where $f(\xi)$ is a solution to $Du'' + Vu' + R(u) = 0$. Linearizing in δu , we obtain the PDE

$$\frac{\partial \delta u}{\partial t} = D \frac{\partial^2 \delta u}{\partial x^2} + R'(u(x - Vt)) \delta u \quad . \quad (6.25)$$

While this equation is linear, it is not autonomous, due to the presence of $u(x - Vt)$ on the in the argument of R' on the right hand side.

Let's shift to a moving frame defined by $\xi = x - Vt$ and $s = t$. Then

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} + \frac{\partial s}{\partial x} \frac{\partial}{\partial s} = \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial t} &= \frac{\partial \xi}{\partial t} \frac{\partial}{\partial \xi} + \frac{\partial s}{\partial t} \frac{\partial}{\partial s} = -V \frac{\partial}{\partial \xi} + \frac{\partial}{\partial s} \quad . \end{aligned} \quad (6.26)$$

So now we have the linear PDE

$$\delta u_s = D \delta u_{\xi\xi} + V \delta u_{\xi} + R'(u(\xi)) \delta u \quad . \quad (6.27)$$

This equation, unlike eqn. 6.25, is linear and autonomous. We can spot one solution immediately. Let $\delta u(\xi, s) = Cu'(\xi)$, where C is a constant. Then the RHS of the above equation is

$$\begin{aligned} \text{RHS} &= D u_{\xi\xi\xi} + V u_{\xi\xi} + R'(u) u_{\xi} \\ &= \frac{d}{d\xi} \left[D u_{\xi\xi} + V u_{\xi} + R(u) \right] = 0 \quad , \end{aligned} \quad (6.28)$$

by virtue of the front equation for $u(\xi)$ itself. This solution is called the *zero mode*. It is easy to understand why such a solution must exist. Due to translation invariance in space and time, if $u(x, t) = u(x - Vt)$ is a solution, then so must $u(x - a, t) = u(x - a - Vt)$ be a solution, and for all values of a . Now differentiate with respect to a and set $a = 0$. The result is the zero mode, $u'(x - Vt)$.

If we define (writing $t = s$)

$$\delta u(\xi, t) = e^{-V\xi/2D} \psi(\xi, t) \quad , \quad (6.29)$$

then we obtain a Schrödinger-like equation for $\psi(\xi, t)$, *i.e.*

$$-\psi_t = \hat{K}\psi \quad , \quad \hat{K} = -D \frac{\partial^2}{\partial \xi^2} + W(\xi) \quad , \quad (6.30)$$

with

$$W(\xi) = \frac{V^2}{4D} - R'(u(\xi)) \quad . \quad (6.31)$$

The Schrödinger equation is separable, so we can write $\psi(\xi, t) = e^{-Et} \phi(\xi)$, obtaining

$$E\phi = -D\phi_{\xi\xi} + W(\xi)\phi \quad . \quad (6.32)$$

Since the zero mode solution $\delta u = u'(\xi)$ is an $E = 0$ solution, and since $u'(\xi)$ must be nodeless, the zero mode energy must be the ground state for this system, and all other eigenvalues must lie at positive energy. This proves that the front solution $u(x - Vt)$ is stable, provided the zero mode lies within the eigenspectrum of eqn. 6.32.

For $\xi \rightarrow -\infty$ we have $u \rightarrow u_L$ with $R'(u_L) < 0$ by assumption. Thus, $W(-\infty) > 0$ and all $E > 0$ solutions are exponentially decaying. As $\xi \rightarrow +\infty$, the solutions decay exponentially if $R'(u_R) < 0$, i.e. if u_R is a stable fixed point of the local dynamics. If on the other hand u_R is an *unstable* fixed point, then $R'(u_R) > 0$. We see immediately that propagation velocities with $V < V_c = 2\sqrt{DR'(u_R)}$ are unstable, since $W(+\infty) < 0$ in such cases. On the other hand, for $V > V_c$, we have that

$$\psi(\xi) = e^{V\xi/2D} \delta u(\xi) \sim A_R \exp\left(\sqrt{V^2 - V_c^2} \xi/2D\right) \quad , \quad (6.33)$$

which is unnormalizable! Hence, the zero mode is no longer part of the eigenspectrum – translational invariance has been lost! One possible resolution is that $V = V_c$, where the threshold of normalizability lies. This is known as the *Fisher velocity*.

6.1.4 Fisher's equation

If we take $R(u) = ru(1 - u)$, the local reaction kinetics are those of the logistic equation $\dot{u} = ru(1 - u)$. With $r > 0$, this system has an unstable fixed point at $u = 0$ and a stable fixed point at $u = 1$. Rescaling time to eliminate the rate constant r , and space to eliminate the diffusion constant D , the corresponding one-dimensional RDE is

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u(1 - u) \quad , \quad (6.34)$$

which is known as Fisher's equation (1937), originally proposed to describe the spreading of biological populations. Note that the physical length scale is $\ell = (D/r)^{1/2}$ and the physical time scale is $\tau = r^{-1}$. Other related RDEs are the Newell-Whitehead Segel equation, for which $R(u) = u(1 - u^2)$, and the Zeldovich equation, for which $R(u) = u(1 - u)(a - u)$ with $0 < a < 1$.

To study front propagation, we assume $u(x, t) = u(x - Vt)$, resulting in

$$\frac{d^2 u}{d\xi^2} + V \frac{du}{d\xi} = -U'(u) \quad , \quad (6.35)$$

where

$$U(u) = -\frac{1}{3}u^3 + \frac{1}{2}u^2 \quad . \quad (6.36)$$

Let $v = du/d\xi$. Then we have the $N = 2$ dynamical system

$$\frac{du}{d\xi} = v \quad , \quad \frac{dv}{d\xi} = -u(1 - u) - Vv \quad , \quad (6.37)$$

with fixed points at $(u^*, v^*) = (0, 0)$ and $(u^*, v^*) = (1, 0)$. The Jacobian matrix is

$$M = \begin{pmatrix} 0 & 1 \\ 2u^* - 1 & -V \end{pmatrix} \quad (6.38)$$

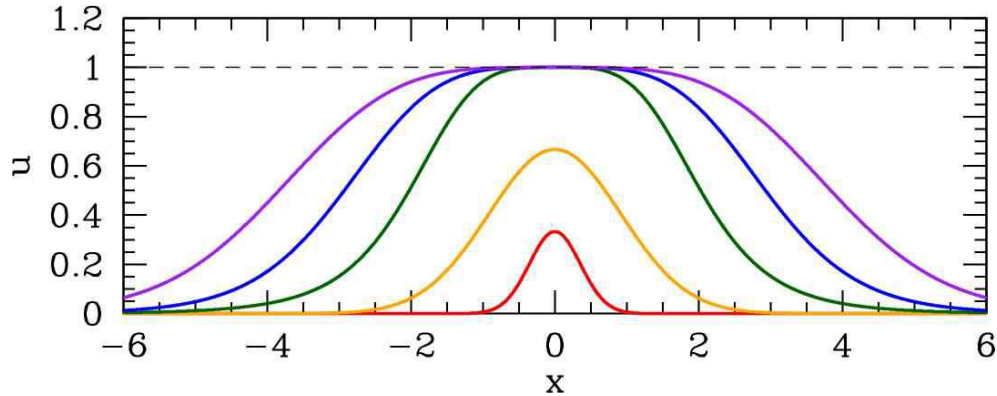


Figure 6.2: Evolution of a blip in the Fisher equation. The initial configuration is shown in red. Progressive configurations are shown in orange, green, blue, and purple. Asymptotically the two fronts move with speed $V = 2$.

At $(u^*, v^*) = (1, 0)$, we have $\det(M) = -1$ and $\text{Tr}(M) = -V$, corresponding to a saddle. At $(u^*, v^*) = (0, 0)$, we have $\det(M) = 1$ and $\text{Tr}(M) = -V$, corresponding to a stable node if $V > 2$ and a stable spiral if $0 < V < 2$. If $u(x, t)$ describes a density, then we must have $u(x, t) \geq 0$ for all x and t , and this rules out $0 < V < 2$ since the approach to the $u^* = 0$ fixed point is oscillating (and damped).

6.1.5 Velocity selection and stability

Is there a preferred velocity V ? According to our analysis thus far, any $V \geq V_c = 2$ will yield an acceptable front solution with $u(x, t) > 0$. However, Kolmogorov and collaborators proved that starting with the initial conditions $u(x, t = 0) = \Theta(-x)$, the function $u(x, t)$ evolves to a traveling wave solution with $V = 2$, which is the minimum allowed propagation speed. That is, the system exhibits *velocity selection*.

We can begin to see why if we assume an asymptotic solution $u(\xi) = A e^{-\kappa\xi}$ as $\xi \rightarrow \infty$. Then since $u^2 \ll u$ we have the linear equation

$$u'' + V u' + u = 0 \quad \Rightarrow \quad V = \kappa + \kappa^{-1} . \quad (6.39)$$

Thus, any $\kappa > 0$ yields a solution, with $V = V(\kappa)$. Note that the minimum allowed value is $V_{\min} = 2$, achieved at $\kappa = 1$. If $\kappa < 1$, the solution falls off more slowly than for $\kappa = 1$, and we apparently have a propagating front with $V > 2$. However, if $\kappa > 1$, the solution decays more rapidly than for $\kappa = 1$, and the $\kappa = 1$ solution will dominate.

We can make further progress by deriving a formal asymptotic expansion. We start with the front equation

$$u'' + V u' + u(1 - u) = 0 , \quad (6.40)$$

and we define $z = \xi/V$, yielding

$$\epsilon \frac{d^2 u}{dz^2} + \frac{du}{dz} + u(1 - u) = 0 , \quad (6.41)$$

with $\epsilon = V^{-2} \leq \frac{1}{4}$. We now develop a perturbation expansion:

$$u(z; \epsilon) = u_0(z) + \epsilon u_1(z) + \dots \quad , \quad (6.42)$$

and isolating terms of equal order in ϵ , we obtain a hierarchy. At order $\mathcal{O}(\epsilon^0)$, we have

$$u_0' + u_0(1 - u_0) = 0 \quad , \quad (6.43)$$

which is to say

$$\frac{du_0}{u_0(u_0 - 1)} = d \ln (u_0^{-1} - 1) = dz \quad . \quad (6.44)$$

Thus,

$$u_0(z) = \frac{1}{\exp(z - a) + 1} \quad , \quad (6.45)$$

where a is a constant of integration. At level k of the hierarchy, with $k > 1$ we have

$$u_{k-1}'' + u_k' + u_k - \sum_{l=0}^k u_l u_{k-l} = 0 \quad , \quad (6.46)$$

which is a first order ODE relating u_k at level k to the set $\{u_j\}$ at levels $j < k$. Separating out the terms, we can rewrite this as

$$u_k' + (1 - 2u_0) u_k = -u_{k-1}'' - \sum_{l=1}^{k-1} u_l u_{k-l} \quad . \quad (6.47)$$

At level $k = 1$, we have

$$u_1' + (1 - 2u_0) u_1 = -u_0'' \quad . \quad (6.48)$$

Plugging in our solution for $u_0(z)$, this inhomogeneous first order ODE may be solved via elementary means. The solution is

$$u_1(z) = -\frac{\ln \cosh\left(\frac{z-a}{2}\right)}{2 \cosh^2\left(\frac{z-a}{2}\right)} \quad . \quad (6.49)$$

Here we have adjusted the constant of integration so that $u_1(a) \equiv 0$. Without loss of generality we may set $a = 0$, and we obtain

$$u(\xi) = \frac{1}{\exp(\xi/V) + 1} - \frac{1}{2V^2} \frac{\ln \cosh(\xi/2V)}{\cosh^2(\xi/2V)} + \mathcal{O}(V^{-4}) \quad . \quad (6.50)$$

At $\xi = 0$, where the front is steepest, we have

$$-u'(0) = \frac{1}{4V} + \mathcal{O}(V^{-3}) \quad . \quad (6.51)$$

Thus, the *slower* the front moves, the *steeper* it gets. Recall that we are assuming $V \geq 2$ here.

6.2 Multi-Species Reaction-Diffusion Systems

We've already introduced the general multi-species RDE,

$$\frac{\partial u_i}{\partial t} = D_{ij} \nabla^2 u_i + R_i(u_1, \dots, u_N) \quad . \quad (6.52)$$

We will be interested in stable traveling wave solutions to these coupled nonlinear PDEs. We'll start with a predator-prey model,

$$\begin{aligned} \frac{\partial N_1}{\partial t} &= rN_1 \left(1 - \frac{N_1}{K}\right) - \alpha N_1 N_2 + D_1 \frac{\partial^2 N_1}{\partial x^2} \\ \frac{\partial N_2}{\partial t} &= \beta N_1 N_2 - \gamma N_2 + D_2 \frac{\partial^2 N_2}{\partial x^2} \quad . \end{aligned} \quad (6.53)$$

Rescaling x , t , N_1 , and N_2 , this seven parameter system can be reduced to one with only three parameters, all of which are assumed to be positive:

$$\begin{aligned} \frac{\partial u}{\partial t} &= u(1 - u - v) + \mathcal{D} \frac{\partial^2 u}{\partial x^2} \\ \frac{\partial v}{\partial t} &= av(u - b) + \frac{\partial^2 v}{\partial x^2} \quad . \end{aligned} \quad (6.54)$$

The interpretation is as follows. According to the local dynamics, species v is parasitic in that it decays as $\dot{v} = -abv$ in the absence of u . The presence of u increases the growth rate for v . Species u on the other hand will grow in the absence of v , and the presence of v decreases its growth rate and can lead to its extinction. Thus, v is the predator and u is the prey.

Before analyzing this reaction-diffusion system, we take the opportunity to introduce some notation on partial derivatives. We will use subscripts to denote partial differentiation, *e.g.*

$$\phi_t = \frac{\partial \phi}{\partial t} \quad , \quad \phi_{xx} = \frac{\partial^2 \phi}{\partial x^2} \quad , \quad \phi_{xxt} = \frac{\partial^3 \phi}{\partial x^2 \partial t} \quad , \quad \text{etc.} \quad (6.55)$$

Thus, our two-species RDE may be written

$$\begin{aligned} u_t &= u(1 - u - v) + \mathcal{D} u_{xx} \\ v_t &= av(u - b) + v_{xx} \quad . \end{aligned} \quad (6.56)$$

We assume $0 < b < 1$, in which case there are three fixed points:

$$\text{empty state: } (u^*, v^*) = (0, 0)$$

$$\text{prey at capacity: } (u^*, v^*) = (1, 0)$$

$$\text{coexistence: } (u^*, v^*) = (b, 1 - b) \quad .$$

We now compute the Jacobian for the local dynamics:

$$M = \begin{pmatrix} \dot{u}_u & \dot{u}_v \\ \dot{v}_u & \dot{v}_v \end{pmatrix} = \begin{pmatrix} 1 - 2u - v & -u \\ av & a(u - b) \end{pmatrix} . \quad (6.57)$$

We now examine the three fixed points.

- At $(u^*, v^*) = (0, 0)$ we have

$$M_{(0,0)} = \begin{pmatrix} 1 & 0 \\ 0 & -b \end{pmatrix} \Rightarrow T = 1 - b \quad , \quad D = -b \quad , \quad (6.58)$$

corresponding to a saddle.

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

$$M_{(1,0)} = \begin{pmatrix} -1 & -1 \\ 0 & a(1 - b) \end{pmatrix} \Rightarrow T = a(1 - b) - 1 \quad , \quad D = -a(1 - b) \quad , \quad (6.59)$$

which is also a saddle, since $0 < b < 1$.

- Finally, at $(u^*, v^*) = (b, 1 - b)$,

$$M_{(b,1-b)} = \begin{pmatrix} -b & -b \\ a(1 - b) & 0 \end{pmatrix} \Rightarrow T = -b \quad , \quad D = ab(1 - b) \quad . \quad (6.60)$$

Since $T < 0$ and $D > 0$ this fixed point is stable. For $D > \frac{1}{4}T^2$ it corresponds to a spiral, and otherwise a node. In terms of a and b , this transition occurs at $a = b/4(1 - b)$. That is,

$$\text{stable node: } a < \frac{b}{4(1 - b)} \quad , \quad \text{stable spiral: } a > \frac{b}{4(1 - b)} . \quad (6.61)$$

The local dynamics has an associated Lyapunov function,

$$L(u, v) = ab \left[\frac{u}{b} - 1 - \ln \left(\frac{u}{b} \right) \right] + (1 - b) \left[\frac{v}{1 - b} - 1 - \ln \left(\frac{v}{1 - b} \right) \right] . \quad (6.62)$$

The constants in the above Lyapunov function are selected to take advantage of the relation $x - 1 - \ln x \geq 0$; thus, $L(u, v) \geq 0$, and $L(u, v)$ achieves its minimum $L = 0$ at the stable fixed point $(b, 1 - b)$. Ignoring diffusion, under the local dynamics we have

$$\frac{dL}{dt} = -a(u - b)^2 \leq 0 \quad . \quad (6.63)$$

6.2.1 Propagating front solutions

We now look for a propagating front solution of the form

$$u(x, t) = u(x - Vt) \quad , \quad v(x, t) = v(x - Vt) \quad . \quad (6.64)$$

This results in the coupled ODE system,

$$\begin{aligned} \mathcal{D} u'' + V u' + u(1 - u - v) &= 0 \\ v'' + V v' + av(u - b) &= 0 \quad , \end{aligned} \quad (6.65)$$

where once again the independent variable is $\xi = x - Vt$. These two coupled second order ODEs may be written as an $N = 4$ system.

We will make a simplifying assumption and take $\mathcal{D} = D_1/D_2 = 0$. This is appropriate if one species diffuses very slowly. An example might be plankton ($D_1 \approx 0$) and an herbivorous species ($D_2 > 0$). We then have $\mathcal{D} = 0$, which results in the $N = 3$ dynamical system,

$$\begin{aligned} \frac{du}{d\xi} &= -V^{-1} u(1 - u - v) \\ \frac{dv}{d\xi} &= w \\ \frac{dw}{d\xi} &= -av(u - b) - Vw \quad , \end{aligned} \quad (6.66)$$

where $w = v'$. In terms of the $N = 3$ phase space $\varphi = (u, v, w)$, the three fixed points are

$$\begin{aligned} (u^*, v^*, w^*) &= (0, 0, 0) \\ (u^*, v^*, w^*) &= (1, 0, 0) \\ (u^*, v^*, w^*) &= (b, 1 - b, 0) \quad . \end{aligned} \quad (6.67)$$

The first two are unstable and the third is stable. We will look for solutions where the stable solution invades one of the two unstable solutions. Since the front is assumed to propagate to the right, we must have the stable solution at $\xi = -\infty$, *i.e.* $\varphi(-\infty) = (b, 1 - b, 0)$. There are then two possibilities: either (i) $\varphi(+\infty) = (0, 0, 0)$, or (ii) $\varphi(+\infty) = (1, 0, 0)$. We will call the former a type-I front and the latter a type-II front.

For our analysis, we will need to evaluate the Jacobian of the system at the fixed point. In general, we have

$$M = \begin{pmatrix} -V^{-1}(1 - 2u^* - v^*) & V^{-1}u^* & 0 \\ 0 & 0 & 1 \\ -av^* & -a(u^* - b) & -V \end{pmatrix} . \quad (6.68)$$

We now evaluate the behavior at the fixed points.

- Let's first look in the vicinity of $\varphi = (0, 0, 0)$. The linearized dynamics then give

$$\frac{d\eta}{d\xi} = M\eta \quad , \quad M = \begin{pmatrix} -V^{-1} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & ab & -V \end{pmatrix} , \quad (6.69)$$

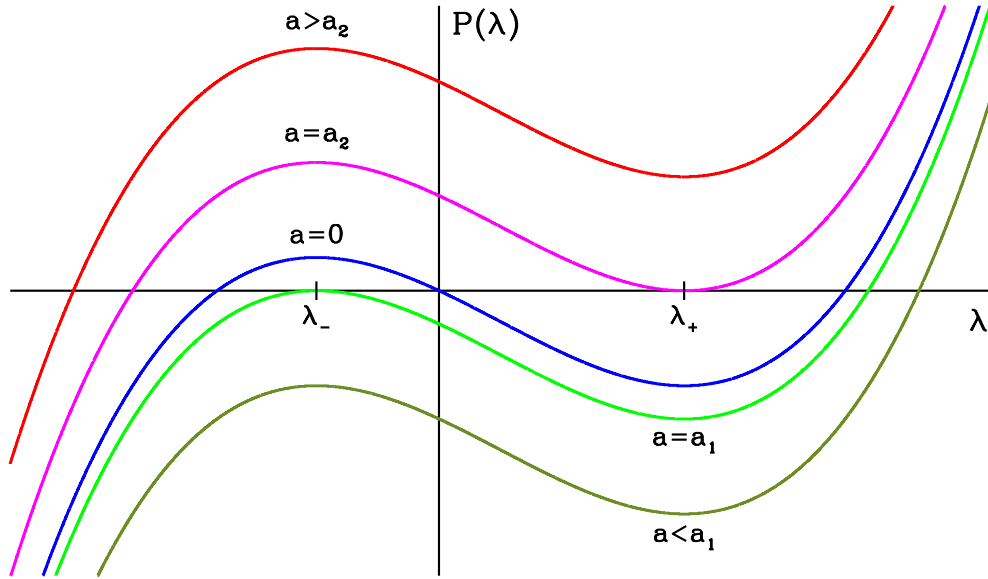


Figure 6.3: Analysis of the characteristic polynomial for the Jacobian of the linearized map at the fixed point $(u^*, v^*, w^*) = (b, 1 - b, 0)$.

where $\varphi = \varphi^* + \eta$. The eigenvalues are

$$\lambda_1 = -V^{-1} \quad , \quad \lambda_{2,3} = -\frac{1}{2}V \pm \frac{1}{2}\sqrt{V^2 + 4ab} \quad . \quad (6.70)$$

We see that $\lambda_{1,2} < 0$ while $\lambda_3 > 0$.

- In the vicinity of $\varphi = (1, 0, 0)$, we have

$$\frac{d\eta}{d\xi} = M\eta \quad , \quad M = \begin{pmatrix} V^{-1} & V^{-1} & 0 \\ 0 & 0 & 1 \\ 0 & a(b-1) & -V \end{pmatrix} \quad , \quad (6.71)$$

The eigenvalues are

$$\lambda_1 = V^{-1} \quad , \quad \lambda_{2,3} = -\frac{1}{2}V \pm \frac{1}{2}\sqrt{V^2 - 4a(1-b)} \quad . \quad (6.72)$$

We now have $\lambda_1 > 0$ and $\text{Re}(\lambda_{2,3}) < 0$. If we exclude oscillatory solutions, then we must have

$$V > V_{\min} = 2\sqrt{a(1-b)} \quad . \quad (6.73)$$

- Finally, let's examine the structure of the fixed point at $\varphi = (b, 1 - b, 0)$, where

$$\frac{d\eta}{d\xi} = M\eta \quad , \quad M = \begin{pmatrix} bV^{-1} & bV^{-1} & 0 \\ 0 & 0 & 1 \\ -a(1-b) & 0 & -V \end{pmatrix} \quad , \quad (6.74)$$

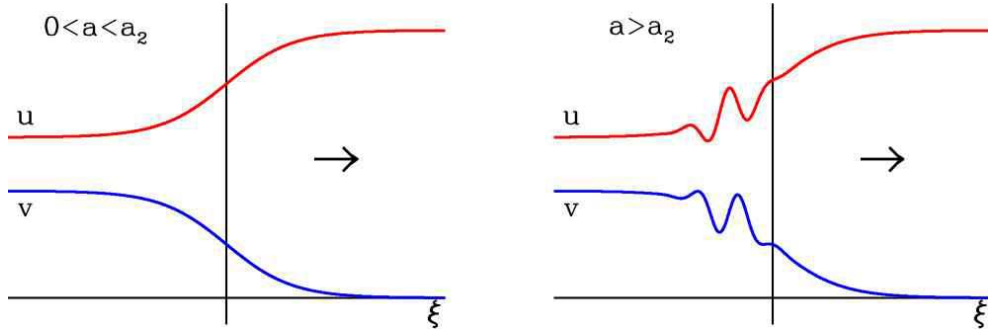


Figure 6.4: Sketch of the type-II front. Left panel: $0 < a < a_2$, for which the trailing edge of the front is monotonic. Right panel: $a > a_2$, for which the trailing edge of the front is oscillatory. In both cases, $\frac{1}{2} < b < 1$, and the front propagates to the right.

The characteristic polynomial is

$$\begin{aligned} P(\lambda) &= \det(\lambda \cdot \mathbb{I} - M) \\ &= \lambda^3 + (V - bV^{-1})\lambda^2 - b\lambda + ab(1-b)V^{-1} \quad . \end{aligned} \quad (6.75)$$

Although physically we want to restrict $a > 0$, we will analyze this cubic for general a , but still $0 < b_1$. First, note that $P(\lambda)$ has extrema when $P'(\lambda) = 0$, which is to say

$$\lambda = \lambda_{\pm} = -\frac{1}{3}(V - bV^{-1}) \pm \frac{1}{3}\sqrt{(V - bV^{-1})^2 + 3b} \quad . \quad (6.76)$$

Note that $\lambda_- < 0 < \lambda_+$. Since the sign of the cubic term in $P(\lambda)$ is positive, we must have that λ_- is a local maximum and λ_+ a local minimum. Note furthermore that both λ_+ and λ_- are independent of the constant a , and depend only on b and c . Thus, the situation is as depicted in fig. 6.3. The constant a merely shifts the cubic $P(\lambda)$ uniformly up or down. When $a = 0$, $P(0) = 0$ and the curve runs through the origin. There exists an $a_1 < 0$ such that for $a = a_1$ we have $P(\lambda_-) = 0$. Similarly, there exists an $a_2 > 0$ such that for $a = a_2$ we have $P(\lambda_+) = 0$. Thus,

$$\begin{aligned} a < a_1 < 0 & : \quad \text{Re}(\lambda_{1,2}) < 0 < \lambda_3 \\ a_1 < a < 0 & : \quad \lambda_1 < \lambda_2 < 0 < \lambda_3 \\ a = 0 & : \quad \lambda_1 < \lambda_2 = 0 < \lambda_3 \\ 0 < a < a_2 & : \quad \lambda_1 < 0 < \lambda_2 < \lambda_3 \\ 0 < a_2 < a & : \quad \lambda_1 < 0 < \text{Re}(\lambda_{2,3}) \quad . \end{aligned} \quad (6.77)$$

Since this is the fixed point approached as $\xi \rightarrow -\infty$, we must approach it along one of its *unstable* manifolds, *i.e.* along a direction corresponding to a positive eigenvalue. Thus, we conclude that if $a > a_2$ that the approach is oscillatory, while for $0 < a < a_2$ the approach is monotonic.

In fig. 6.4 we sketch the solution for a type-II front, where the stable coexistence phase invades the unstable ‘prey at capacity’ phase.

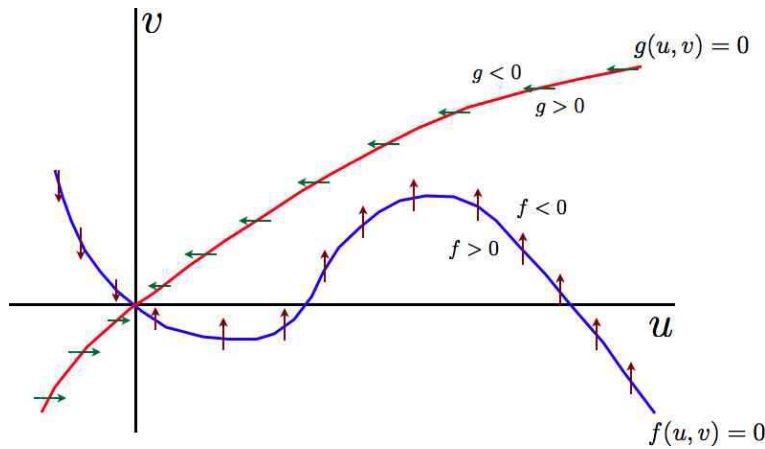


Figure 6.5: Sketch of the nullclines for the dynamical system described in the text.

6.3 Excitable Media

Consider the following $N = 2$ system:

$$\begin{aligned}\dot{u} &= f(u, v) \\ \dot{v} &= \epsilon g(u, v) \quad ,\end{aligned}\tag{6.78}$$

where $0 < \epsilon \ll 1$. The first equation is ‘fast’ and the second equation ‘slow’. We assume the nullclines for $f = 0$ and $g = 0$ are as depicted in fig. 6.5. As should be clear from the figure, the origin is a stable fixed point. In the vicinity of the origin, we can write

$$\begin{aligned}f(u, v) &= -au - bv + \dots \\ g(u, v) &= +cu - dv + \dots \quad ,\end{aligned}\tag{6.79}$$

where a, b, c , and d are all positive real numbers. The equation for the nullclines in the vicinity of the origin is then $au + bv = 0$ for the $f = 0$ nullcline, and $cu - dv = 0$ for the $g = 0$ nullcline. Note that

$$M \equiv \left. \frac{\partial(\dot{u}, \dot{v})}{\partial(u, v)} \right|_{(0,0)} = \begin{pmatrix} -a & -b \\ \epsilon c & -\epsilon d \end{pmatrix} \quad .\tag{6.80}$$

We then have $\text{Tr } M = -(a + \epsilon d) < 0$ and $\det M = \epsilon(ad + bc) > 0$. Since the trace is negative and the determinant positive, the fixed point is stable. The boundary between spiral and node solutions is $\det M = \frac{1}{4}(\text{Tr } M)^2$, which means

$$\begin{aligned}|a - \epsilon d| &> 2\sqrt{\epsilon bc} \quad : \text{ stable node} \\ |a - \epsilon d| &< 2\sqrt{\epsilon bc} \quad : \text{ stable spiral} \quad .\end{aligned}\tag{6.81}$$

Although the trivial fixed point $(u^*, v^*) = (0, 0)$ is stable, it is still *excitable* in the sense that a large enough perturbation will result in a big excursion. Consider the sketch in fig. 6.6. Starting from A, v initially increases as u decreases, but eventually both u and v get sucked into the stable fixed point at

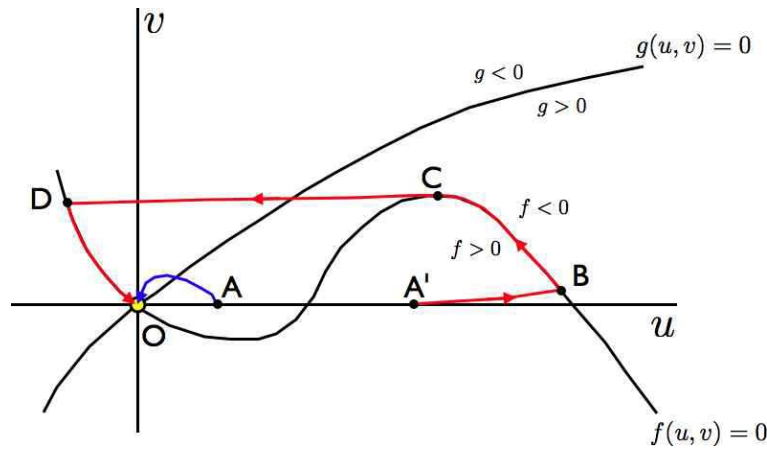


Figure 6.6: Sketch of the fizzle, which starts from A, and the burst, which starts from A'.

O. We call this path the *fizzle*. Starting from A', however, u begins to increase rapidly and v increases slowly until the $f = 0$ nullcline is reached. At this point the fast dynamics has played itself out. The phase curve follows the nullcline, since any increase in v is followed by an immediate readjustment of u back to the nullcline. This state of affairs continues until C is reached, at which point the phase curve makes a large rapid excursion to D, following which it once again follows the $f = 0$ nullcline to the origin O. We call this path a *burst*. The behavior of $u(t)$ and $v(t)$ during these paths is depicted in fig. 6.7.

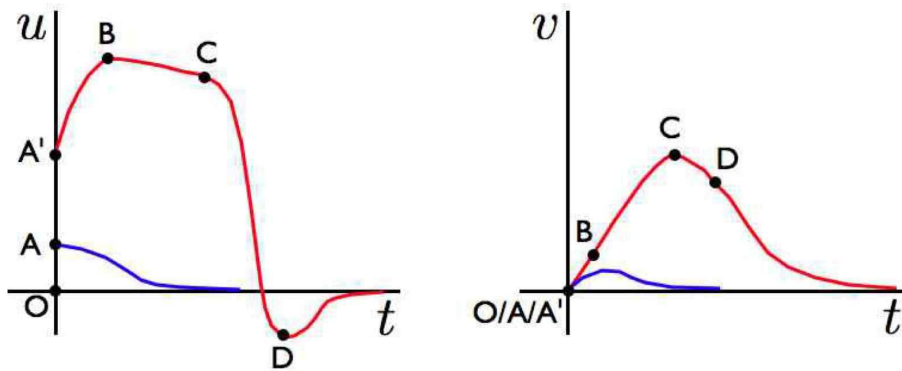


Figure 6.7: Sketch of $u(t)$ and $v(t)$ for the fizzle and burst.

It is also possible for there to be multiple bursts. Consider for example the situation depicted in fig. 6.8, in which the $f = 0$ and $g = 0$ nullclines cross three times. Two of these crossings correspond to stable (attractive) fixed points, while the third is unstable. There are now two different large scale excursion paths, depending on which stable fixed point one ends up at¹.

¹For a more egregious example of a sentence ending in several prepositions: "What did you bring that book I didn't want to be read to out of up around for?"

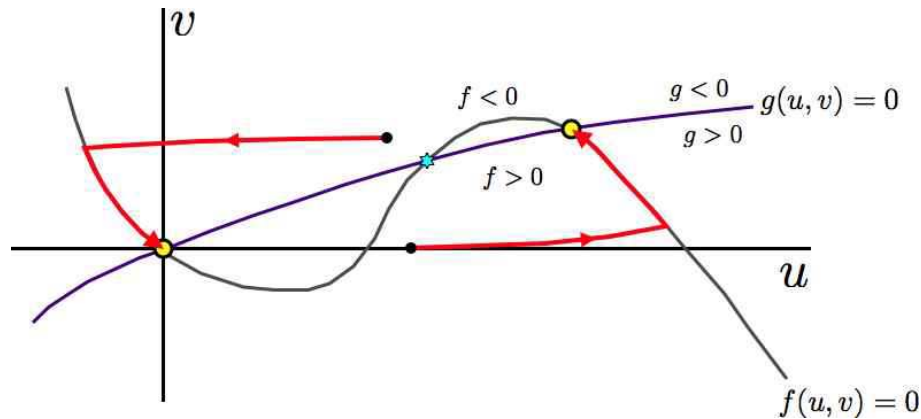


Figure 6.8: With three nullcline crossings, there are two stable fixed points, and hence two types of burst. The yellow-centered circles denote stable fixed points, and the blue-centered star denotes an unstable fixed point.

6.3.1 Front propagation in excitable media

Now let's add in diffusion:

$$\begin{aligned} u_t &= D_1 u_{xx} + f(u, v) \\ v_t &= D_2 v_{xx} + \epsilon g(u, v) \end{aligned} \quad (6.82)$$

We will consider a specific model,

$$\begin{aligned} u_t &= u(a - u)(u - 1) - v + D u_{xx} \\ v_t &= b u - \gamma v \end{aligned} \quad (6.83)$$

This is known as the *FitzHugh-Nagumo model* of nerve conduction (1961-2). It represents a tractable simplification and reduction of the famous Hodgkin-Huxley model (1952) of electrophysiology. Very briefly, u represents the membrane potential, and v the contributions to the membrane current from Na^+ and K^+ ions. We have $0 < a < 1$, $b > 0$, and $\gamma > 0$. The nullclines for the local dynamics resemble those in fig. 6.5, with the nullcline for the slow reaction perfectly straight.

We are interested in wave (front) solutions, which might describe wave propagation in muscle (*e.g.* heart) tissue. Let us once again define $\xi = x - Vt$ and assume a propagating front solution. We then arrive at the coupled ODEs,

$$\begin{aligned} D u'' + V u' + h(u) - v &= 0 \\ V v' + b u - \gamma v &= 0 \end{aligned} \quad (6.84)$$

where

$$h(u) = u(a - u)(u - 1) \quad (6.85)$$

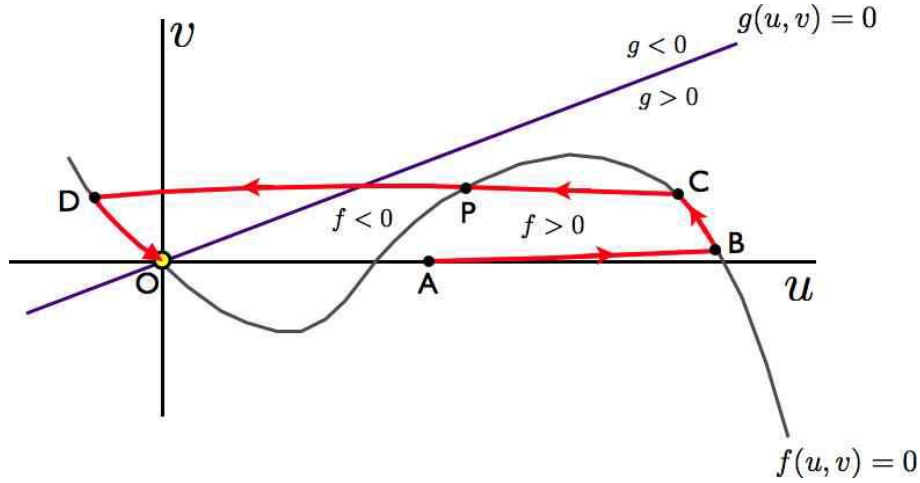


Figure 6.9: Excitation cycle for the FitzHugh-Nagumo model.

Once again, we have an $N = 3$ dynamical system:

$$\begin{aligned} \frac{du}{d\xi} &= w \\ \frac{dv}{d\xi} &= -bV^{-1}u + \gamma V^{-1}v \\ \frac{dw}{d\xi} &= -D^{-1}h(u) + D^{-1}v - VD^{-1}w \quad , \end{aligned} \quad (6.86)$$

where $w = u'$.

We assume that b and γ are both small, so that the v dynamics are slow. Furthermore, v remains small throughout the motion of the system. Then, assuming an initial value $(u_0, 0, 0)$, we may approximate

$$u_t \approx D u_{xx} + h(u) \quad . \quad (6.87)$$

With $D = 0$, the points $u = 1$ and $u = 1$ are both linearly stable and $u = a$ is linearly unstable. For finite D there is a wave connecting the two stable fixed points with a unique speed of propagation.

The equation $Du'' + Vu' = -h(u)$ may again be interpreted mechanically, with $h(u) = U'(u)$. Then since the cubic term in $h(u)$ has a negative sign, the potential $U(u)$ resembles an inverted asymmetric double well, with local maxima at $u = 0$ and $u = 1$, and a local minimum somewhere in between at $u = a$. Since

$$U(0) - U(1) = \int_0^1 du h(u) = \frac{1}{12}(1 - 2a) \quad , \quad (6.88)$$

hence if $V > 0$ we must have $a < \frac{1}{2}$ in order for the left maximum to be higher than the right maximum. The constant V is adjusted so as to yield a solution. This entails

$$V \int_{-\infty}^{\infty} d\xi u_\xi^2 = V \int_0^1 du u_\xi = U(0) - U(1) \quad . \quad (6.89)$$

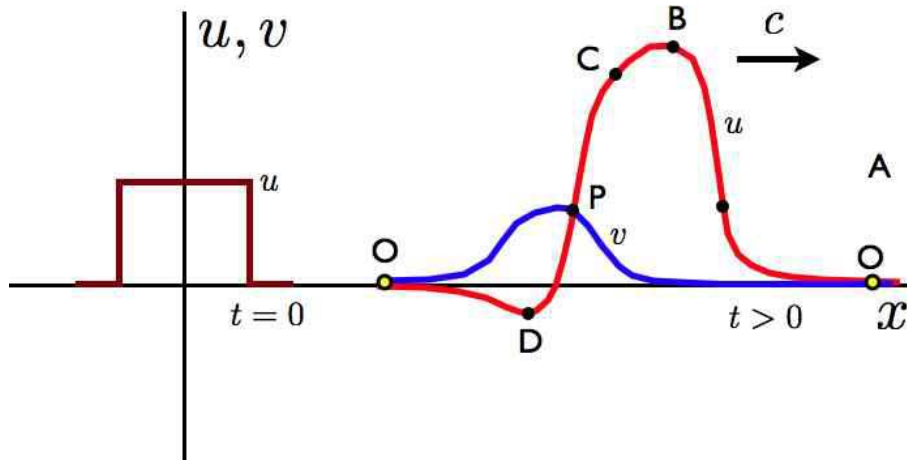


Figure 6.10: Sketch of the excitation pulse of the FitzHugh-Nagumo model.

The solution makes use of some very special properties of the cubic $h(u)$ and is astonishingly simple:

$$V = (D/2)^{1/2} (1 - 2a) \quad . \quad (6.90)$$

We next must find the speed of propagation on the CD leg of the excursion. There we have

$$u_t \approx D u_{xx} + h(u) - v_C \quad , \quad (6.91)$$

with $u(-\infty) = u_D$ and $u(+\infty) = u_C$. The speed of propagation is

$$\tilde{V} = (D/2)^{1/2} (u_C - 2u_P + u_D) \quad . \quad (6.92)$$

We then set $V = \tilde{V}$ to determine the location of C. The excitation pulse is sketched in fig. 6.10

Calculation of the wave speed

Consider the second order ODE,

$$\mathcal{L}(u) \equiv D u'' + V u' + A(u - u_1)(u_2 - u)(u - u_3) = 0 \quad . \quad (6.93)$$

We assume $u_{1,2,3}$ are all distinct. Remarkably, a solution may be found. We claim that if

$$u' = \lambda(u - u_1)(u - u_2) \quad , \quad (6.94)$$

then, by suitably adjusting λ , the solution to eqn. 6.94 also solves eqn. 6.93. To show this, note that under the assumption of eqn. 6.94 we have

$$\begin{aligned} u'' &= \frac{du'}{du} \cdot \frac{du}{d\xi} \\ &= \lambda(2u - u_1 - u_2) u' \\ &= \lambda^2(u - u_1)(u - u_2)(2u - u_1 - u_2) \quad . \end{aligned} \quad (6.95)$$

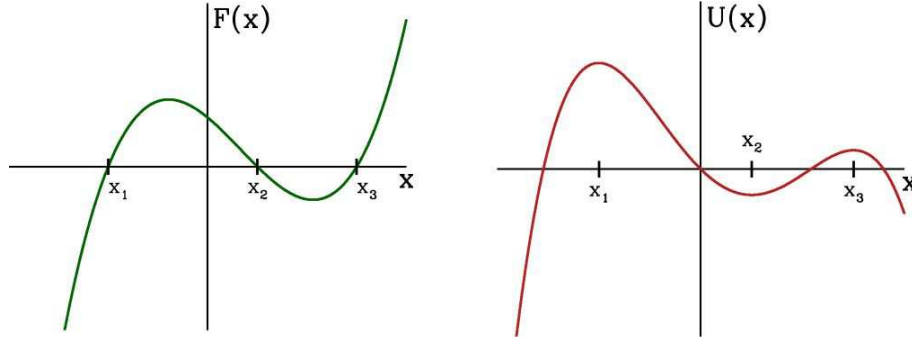


Figure 6.11: Mechanical analog for the front solution, showing force $F(x)$ and corresponding potential $U(x)$.

Thus,

$$\begin{aligned} \mathcal{L}(u) &= (u - u_1)(u - u_2) \left[\lambda^2 D(2u - u_1 - u_2) + \lambda V + A(u_3 - u) \right] \\ &= (u - u_1)(u - u_2) \left[(2\lambda^2 D - A)u + (\lambda V + Au_3 - \lambda^2 D(u_1 + u_2)) \right] . \end{aligned} \quad (6.96)$$

Therefore, if we choose

$$\lambda = \sigma \sqrt{\frac{A}{2D}} \quad , \quad V = \sigma \sqrt{\frac{AD}{2}} (u_1 + u_2 - 2u_3) \quad , \quad (6.97)$$

with $\sigma = \pm 1$, we obtain a solution to $\mathcal{L}(u) = 0$. Note that the velocity V has been *selected*.

The integration of eqn. 6.94 is elementary, yielding the kink solution

$$\begin{aligned} u(\xi) &= \frac{u_2 + u_1 \exp[\lambda(u_2 - u_1)(\xi - \xi_0)]}{1 + \exp[\lambda(u_2 - u_1)(\xi - \xi_0)]} \\ &= \frac{1}{2}(u_1 + u_2) + \frac{1}{2}(u_1 - u_2) \tanh \left[\frac{1}{2} \lambda (u_2 - u_1) (\xi - \xi_0) \right] \quad , \end{aligned} \quad (6.98)$$

where ξ_0 is a constant which is the location of the center of the kink. This front solution connects $u = u_1$ and $u = u_2$. There is also a front solution connecting u_1 and u_3 :

$$u(\xi) = \frac{1}{2}(u_1 + u_3) + \frac{1}{2}(u_1 - u_3) \tanh \left[\frac{1}{2} \lambda (u_3 - u_1) (\xi - \xi_0) \right] \quad , \quad (6.99)$$

with the same value of $\lambda = \sigma \sqrt{A/2D}$, but with a different velocity of front propagation, given by $V = \sigma(AD/2)^{1/2}(u_1 + u_3 - 2u_2)$, again with $\sigma = \pm 1$.

It is instructive to consider the analogue mechanical setting of eqn. 6.93. We write $D \rightarrow M$ and $V \rightarrow \gamma$, and $u \rightarrow x$, giving

$$M\ddot{x} + \gamma\dot{x} = A(x - x_1)(x - x_2)(x - x_3) \equiv F(x) \quad , \quad (6.100)$$

where we take $x_1 < x_2 < x_3$. Mechanically, the points $x = x_{1,3}$ are unstable equilibria. A front solution interpolates between these two stationary states. If $\gamma = V > 0$, the friction is of the usual sign, and the

path starts from the equilibrium at which the potential $U(x)$ is greatest. Note that

$$U(x_1) - U(x_3) = \int_{x_1}^{x_3} dx F(x) = \frac{1}{12}(x_3 - x_1)^2 \left[(x_2 - x_1)^2 - (x_3 - x_2)^2 \right] . \quad (6.101)$$

so if, for example, the integral of $F(x)$ between x_1 and x_3 is positive, then $U(x_1) > U(x_3)$. For our cubic force $F(x)$, this occurs if $x_2 > \frac{1}{2}(x_1 + x_3)$.