Waves in Reaction-Diffusion Systems

We've studied simple dynamical systems of the form

$$\frac{du}{dt} = f(u)$$

The dynamics evolves $u(t)$ toward the first stable fixed point encountered. Now let's add diffusion:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u)$$

We'll look for traveling wave sol$^{\underline{ns}}$ of the form

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

$$\xi \equiv x - vt$$

so the PDE becomes an ODE:

$$D\frac{d^2u}{d\xi^2} + v\frac{du}{d\xi} + f(u) = 0$$

Consider first

$$f(u) = \gamma u(1-u)$$

$$\Rightarrow \quad \frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + \gamma u(1-u)$$

which is known as the Fisher eqn.

We adimensionalize by

$$t \to \gamma t \quad , \quad x \to (\gamma/D)^{1/2} x$$

whence we obtain

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

With the Ansatz $u(x,t) = u(x-ct)$, we have

$$\frac{d^2u}{d\xi^2} + c\frac{du}{d\xi} + u(1-u) = 0$$

Let $w \equiv \frac{du}{d\xi}$. Then

$$\frac{d}{d\xi}\begin{pmatrix} u \\ w \end{pmatrix} = \begin{pmatrix} w \\ -cw - u(1-u) \end{pmatrix}$$

We analyze this in the usual way. Fixed points lie at

$$\begin{pmatrix} u^* \\ w^* \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad , \quad \begin{pmatrix} u^* \\ w^* \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

Linearization:

$$\begin{matrix} u = \delta u \\ w = \delta w \end{matrix} \quad \Rightarrow \quad \frac{d}{d\xi}\begin{pmatrix} \delta u \\ \delta w \end{pmatrix} = \overbrace{\begin{pmatrix} 0 & 1 \\ -1 & -c \end{pmatrix}}^{M}\begin{pmatrix} \delta u \\ \delta w \end{pmatrix}$$

$$\mathrm{Tr}\, M = -c \,, \quad \det M = +1 \,, \quad \lambda_\pm = \frac{1}{2}\left\{-c \pm \sqrt{c^2-4}\right\}$$

$c < -2$: unstable node ; $-2 < c < 0$: unstable spiral

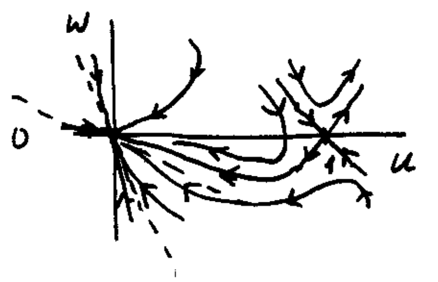
$c > +2$: stable node ; $0 < c < 2$: stable spiral

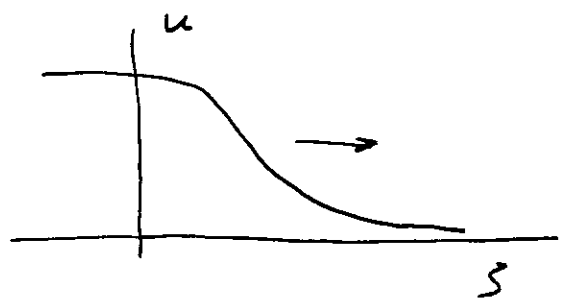
$$\left.\begin{array}{l} u = 1+\delta u \\ w = \delta w \end{array}\right\} \Rightarrow \frac{d}{d\xi}\begin{pmatrix}\delta u \\ \delta w\end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & -c \end{pmatrix}\begin{pmatrix}\delta u \\ \delta w\end{pmatrix}$$

$$\operatorname{Tr} M = -c \ , \quad \det M = -1 \ , \quad \lambda_\pm = \tfrac{1}{2}\left\{-c \pm \sqrt{c^2+4}\right\}$$

$\Rightarrow$ saddle (all values of c)

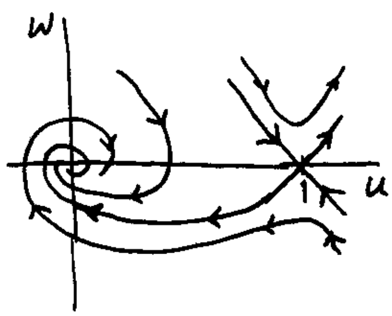
For $c \geq 2$ then,

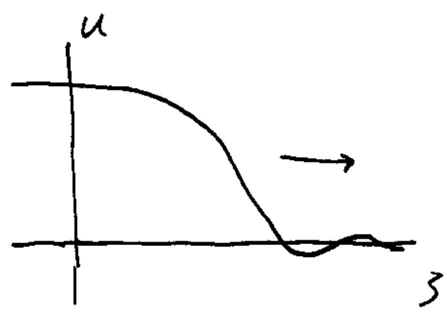




I.e. there exists a sol^{n} connecting the two FPs.

For $0 < c < 2$,





If u represents a density, this latter sol^{n} is unphysical.

Is there any preferred velocity? Kolmogorov et al. (1937) proved that if

$$u(x,0) = u_0(x) > 0 \qquad \begin{array}{ll} u_0(x) = 1 & \text{for } x < x_1 \\ u_0(x) = 0 & \text{for } x > x_2 \end{array}$$

that $u(x,t)$ evolves to a travelling wavefront sol$^{\underline{n}}$ with $c=2$. I.e. minimum speed.

Suppose that as $\xi \to \infty$ we have

$$u(\xi) = A e^{-K\xi}$$

Then assuming $u^2 \ll u$, we have

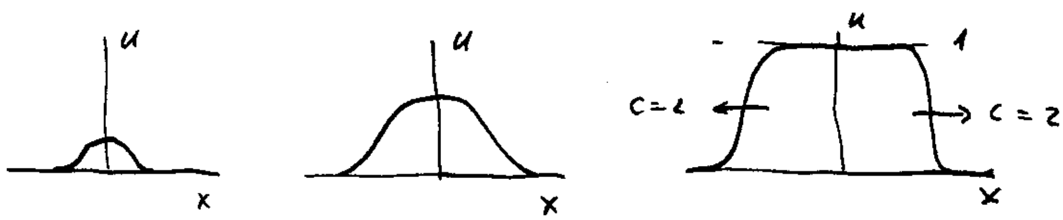
$$u'' + cu' + u = 0$$

$$\Rightarrow \quad c = K + K^{-1}$$

Note $c_{min} = 2$, at $K=1$. If $K<1$, $c = K + K^{-1} > 2$, but if $K>1$, we have that $e^{-K\xi}$ is bounded above by the $K=1$ sol$^{\underline{n}}$, $e^{-\xi}$, which has velocity $c=2$. Thus,

$$0 < K \leq 1 \ : \quad c = K + K^{-1} \quad ; \quad K \geq 1 \ : \quad c = 2$$

Evolution of a blip:



Asymptotic Sol$^{\underline{n}}$

Start with

$$\frac{d^2u}{d\xi^2} + c\frac{du}{d\xi} + u(1-u) = 0$$

and write

$$u(\xi) \equiv g(z = \xi/c)$$

$$\Rightarrow \quad \frac{1}{c^2}\frac{d^2g}{dz^2} + \frac{dg}{dz} + g(1-g) = 0$$

Define $\epsilon \equiv c^{-2} \leq \frac{1}{4}$. Perturbation expansion:

$$g(z;\epsilon) = g_0(z) + \epsilon g_1(z) + \cdots$$

$$① \quad g_0' + g_0(1-g_0) = 0$$

$$② \quad g_0'' + g_1' + (1-2g_0)g_1 = 0$$

etc.

$$g_0' = g_0^2 - g_0$$
$$g_0'' = (2g_0-1)g_0'$$

Thus,

$$-\frac{dg_0}{g_0(1-g_0)} = d\ln(g_0^{-1}-1) = dz$$

and we find

$$g_0(z) = \left\{1+e^{(z-z_0)}\right\}^{-1}$$

At the next level,

$$g_1' = -g_0'' - (1-2g_0)g_1 = -g_0'' + \frac{g_0''}{g_0'}\, g_1$$

$$\Rightarrow \quad g_1 = -g_0' \ln\left(4|g_0'|\right) = \frac{e^{(z-z_0)}}{\left(1+e^{(z-z_0)}\right)^2} \ln\left\{\frac{4e^{(z-z_0)}}{\left(1+e^{(z-z_0)}\right)^2}\right\}$$

constant adjusted

$$= \frac{1}{2}\operatorname{sech}^2\left(\frac{z-z_0}{2}\right) \ln \operatorname{sech}\left(\frac{z-z_0}{2}\right)$$

$$= -\frac{1}{2}\, \frac{\ln\cosh\left(\frac{z-z_0}{2}\right)}{\cosh^2\left(\frac{z-z_0}{2}\right)}$$

Thus,

$$u(\xi) = \frac{1}{1+e^{\xi/c}} - \frac{1}{2c^2}\, \frac{\ln\cosh(\xi/2c)}{\cosh^2(\xi/2c)} + \dots$$

setting $z_0 = 0$. We need $c > 2$ here. At $\xi = 0$,

$$-u'(0) = \frac{1}{4c} + O(1/c^3)$$

Thus, the slower the front moves, the steeper it gets.

(Kolmogorov :  evolves to minimum $c=2$)

Stability

Let's write

$$u(x,t) = u_c(x-ct) + \delta u(x,t)$$

where $u_c(\xi)$ solves $u_c'' + cu_c' + u(1-u) = 0$. The eqn for δu is

$$\frac{\partial}{\partial t}\delta u = \frac{\partial^2}{\partial x^2}\delta u + (1-2u_c)\delta u$$

If we shift to the moving frame with

$$\begin{aligned} \xi &= x-ct \\ t' &= t \end{aligned} \quad \Bigg\} \quad \begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \frac{\partial t'}{\partial x}\frac{\partial}{\partial t'} = \frac{\partial}{\partial \xi} \\ \frac{\partial}{\partial t} &= \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} + \frac{\partial t'}{\partial t}\frac{\partial}{\partial t'} = \frac{\partial}{\partial t'} - c\frac{\partial}{\partial \xi} \end{aligned}$$

Dropping the prime,

$$\frac{\partial \delta u}{\partial t} = \frac{\partial^2 \delta u}{\partial \xi^2} + c\frac{\partial \delta u}{\partial \xi} + (1-2u_c(\xi))\delta u$$

This eqn is linear and autonomous, so look for sol$^{=s}$

$$\delta u(\xi,t) = f(\xi)e^{-\lambda t}$$

$$\Rightarrow \quad f'' + cf' + \{\lambda + 1 - 2u_c(\xi)\} f = 0$$

This is an eigenvalue eqn for λ. Need boundary conditions, which may be taken as $f(\pm\infty) = 0$ or $f(\pm L) = 0$ to 'quantize in a box'. Note that $f(\xi) = u_c'(\xi)$ is an eigenfunction with $\lambda = 0$. This is because

$$u_c(\xi + \delta\xi) = u_c(\xi) + u_c'(\xi)\delta\xi$$

is a sol$^{=}$ due to translational invariance. Finally, writing

$$f(\xi) \equiv h(\xi)\, e^{-c\xi/2}$$

we obtain

$$h'' + \left\{ \lambda - \left(2u_c(\xi) + \frac{c^2}{4} - 1\right) \right\} h = 0$$

$$2u_c(\xi) + \frac{c^2}{4} - 1 \geqslant 2u_c(\xi) > 0$$

Thus, $\lambda_i > 0$ for all i (box quantization) and the sol$^{=}$ is <u>stable</u>.

Multi-species Reaction-Diffusion Models

General form:

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

u_i = vector of reactants
f_i = nonlinear reaction kinetics
D_{ij} = diffusivity matrix

We're interested (usually) in stable, traveling wave sol$^{\text{ns}}$.
Start with a predator-prey model,

$$\frac{\partial u}{\partial t} = u(1-u-v) + D \frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial v}{\partial t} = a v(u-b) + \frac{\partial^2 v}{\partial x^2}$$

which is a rescaled version of

$$\frac{\partial U}{\partial t} = AU\left(1-\frac{U}{K}\right) - BUV + D_1 \nabla^2 U$$

$$\frac{\partial V}{\partial t} = CUV - DV + D_2 \nabla^2 V$$

in $d=1$. Interpretation: V is parasitic; if $U=0$, $V \to 0$. U achieves equilibrium value $U=K$ in absence of V, but is diminished by finite V. Thus, U = prey, V = predator.

$$u_t = u(1-u-v) + Du_{xx}$$
$$v_t = av(u-b) + v_{xx}$$

Steady states:

$(0,0)$	trivial empty state	
$(1,0)$	prey at capacity	
$(b, 1-b)$	coexistence	(assume $0<b<1$)

Matrix of derivatives:

$$\begin{pmatrix} \frac{\partial \dot{u}}{\partial u} & \frac{\partial \dot{u}}{\partial v} \\ \frac{\partial \dot{v}}{\partial u} & \frac{\partial \dot{v}}{\partial v} \end{pmatrix} = \begin{pmatrix} 1-2u-v & -u \\ av & a(u-b) \end{pmatrix} \equiv M$$

Thus

$$M_{(0,0)} = \begin{pmatrix} 1 & 0 \\ 0 & -b \end{pmatrix} \qquad \text{saddle}$$

$$M_{(1,0)} = \begin{pmatrix} -1 & -1 \\ 0 & a(1-b) \end{pmatrix} \qquad \text{saddle (since } b<1)$$

$$M_{(b,1-b)} = \begin{pmatrix} -b & -b \\ a(1-b) & 0 \end{pmatrix} \qquad \begin{array}{l} D \equiv \det M = ab(1-b) \\ T \equiv \mathrm{Tr}\, M = -b < 0 \end{array}$$

$4D > T^2$: stable spiral $\Rightarrow$ $a > \frac{b}{4(1-b)}$

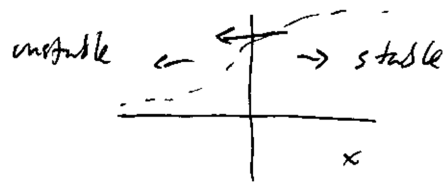
$4D < T^2$: stable node $\Rightarrow$ $a < \frac{b}{4(1-b)}$

Lyapunov f^2:

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

$$\frac{dL}{dt} \leqslant 0 \quad \text{for } u>0,\ v>0$$

Now look for travelling wave sol$^{\underline{n}}$:



$$u(x,t) = \mathbf{u}(x+ct) = u(\xi)$$
$$v(x,t) = v(x+ct) = v(\xi)$$

$$+cu' = u(1-u-v) + Du''$$
$$+cv' = av(u-b) + v''$$

This may be written as a four-dimensional flow

$$\frac{d}{d\xi}\begin{pmatrix} u \\ v \\ u' \\ v' \end{pmatrix} = \begin{pmatrix} u' \\ v' \\ +\frac{c}{D}u' - \frac{u}{D}(1-u-v) \\ +cv' - av(u-b) \end{pmatrix}$$

Simpler case: $D = D_1/D_2 = 0$ -- think plankton ($D_1 = 0$) + herbivore ($D_2 \neq 0$).
Then we have a three-dim'l system:

$$\frac{d}{d\xi}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} +u(1-u-v)/c \\ w \\ +cw - av(u-b) \end{pmatrix}$$

with $w = v'$.

$(0,0,0)$ unstable

$(1,0,0)$ unstable

$(b,1-b,0)$ stable

So look for solns between $(0,0,0)$ and $(b,1-b,0)$
or between $(1,0,0)$ and $(b,1-b,0)$.

$$\frac{d}{d\xi}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} +u(1-u-v)/c \\ w \\ +cw - av(u-b) \end{pmatrix}$$

Two possibilities:

(i) $u(-\infty) = 1$, $v(-\infty) = 0$, $w(-\infty) = 0$

$u(+\infty) = b$, $v(+\infty) = 1-b$, $w(+\infty) = 0$

(ii) $u(-\infty) = 0$, $v(-\infty) = 0$, $w(-\infty) = 0$

$u(+\infty) = b$, $v(+\infty) = 1-b$, $w(+\infty) = 0$

Consider case (i). The linearized dynamics at $(1,0,0)$ are

$$\begin{aligned} \delta u' &= -\delta u/c \\ \delta v' &= \delta w \\ \delta w' &= c\,\delta w - a(1-b)\,\delta v \end{aligned}$$

The eigenvalues of the linearized dynamics are given by $P(\lambda) = 0$,

$$P(\lambda) = \det\begin{pmatrix} \lambda + \frac{1}{c} & 0 & 0 \\ 0 & \lambda & -1 \\ 0 & +a(1-b) & \lambda - c \end{pmatrix}$$

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

Again we require $0 < b < 1$, $a > 0$. The unstable manifold is the (2,3) eigenspace. If we refuse to allow oscillatory sol$^{\underline{ns}}$, then

$$c \geq c_{min} = \sqrt{4a(1-b)}$$

Now let's look in the vicinity of $(b, 1-b, 0)$, where

$$\delta u' = -\frac{b}{c}\,\delta u - \frac{b}{c}\,\delta v$$

$$\delta v' = \delta w$$

$$\delta w' = -a(1-b)\,\delta u + c\,\delta w$$

We now obtain

$$P(\lambda) = \lambda^3 - \lambda^2\left(c - \frac{b}{c}\right) - \lambda b - \frac{ab(1-b)}{c}$$

To analyze this, note

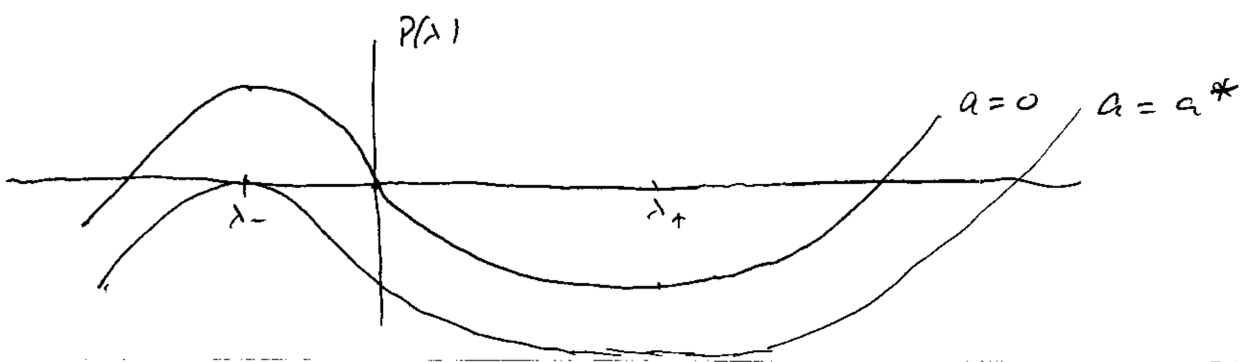
$$p'(\lambda) = 3\lambda^2 - 2\lambda\left(c - \frac{b}{c}\right) - b$$

so

$$p'(\lambda) = 0 \implies \lambda = \lambda_\pm = \frac{\left(c - \frac{b}{c}\right) \pm \sqrt{\left(c - \frac{b}{c}\right)^2 + 3b}}{3}$$

Note $\lambda_\pm$ are independent of a. For $a = 0$, the roots of $P(\lambda) = 0$ are

$$\lambda_1 = 0 \quad , \quad \lambda_{2,3} = \frac{\left(c - \frac{b}{c}\right) \pm \sqrt{\left(c - \frac{b}{c}\right)^2 + 4b}}{2}$$



Thus, defining a^* by $P(\lambda_-)\big|_{a=a^*} = 0$, we see

$a > a^*$: $\lambda_{1,2} = -\alpha \pm i\beta$, $\lambda_3 = +\gamma$

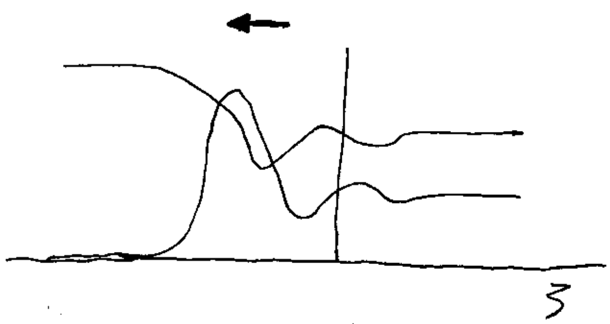
$0 < a < a^*$: $\lambda_1 < \lambda_2 < 0$, $\lambda_3 > 0$

$P(\lambda_+)\big|_{a^{**}} = 0$

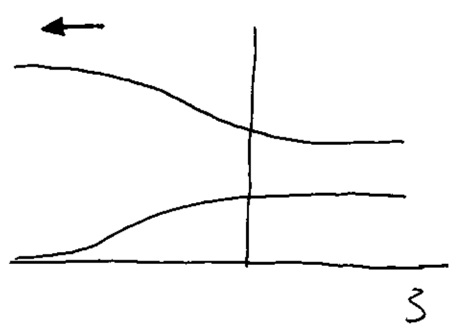
$a^{**} < a < 0$: $\lambda_1 < 0$, $0 < \lambda_2 < \lambda_3$

$a < a^{**}$: $\lambda_1 < 0$, $\lambda_{2,3} = \tilde{\alpha} \pm i\tilde{\beta}$

Thus, if $a > a^*$, sol$^{\underline{ns}}$ approach $(b, 1-b, 0)$ in an oscillatory manner. Note also: this FP is never totally unstable.



$a > a^*$



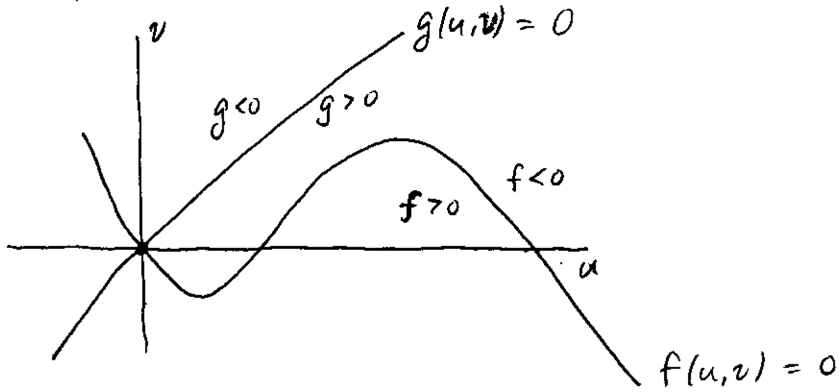
$a < a^*$

Excitable Media

Consider the following system:

$$\dot{u} = f(u,v)$$
$$\dot{v} = \epsilon g(u,v) \qquad \epsilon \ll 1 \Rightarrow v \text{ is "slow"}$$

We now sketch the nullclines $\dot{u}=0$ and $\dot{v}=0$ in the (u,v) plane:



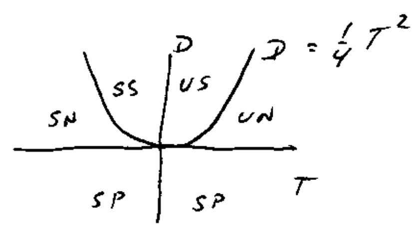
On $f(u,v)=0$, the flow is along $\hat{v}$; along $g(u,v)=0$ the flow is along $\hat{u}$. Note that the origin is stable. In the vicinity of the origin ($\equiv S$), we have

$$f(u,v) \approx -au - bv \qquad a>0,\ b>0$$
$$g(u,v) \approx cu - dv \qquad c>0,\ d>0$$

so that $f(u,v)=0 \Rightarrow v = -\frac{a}{b}u$; $g(u,v)=0 \Rightarrow v = +\frac{c}{d}u$.

Then

$$\frac{\partial(f,g)}{\partial(u,v)} = \begin{pmatrix} -a & -b \\ c & -d \end{pmatrix} \equiv M$$



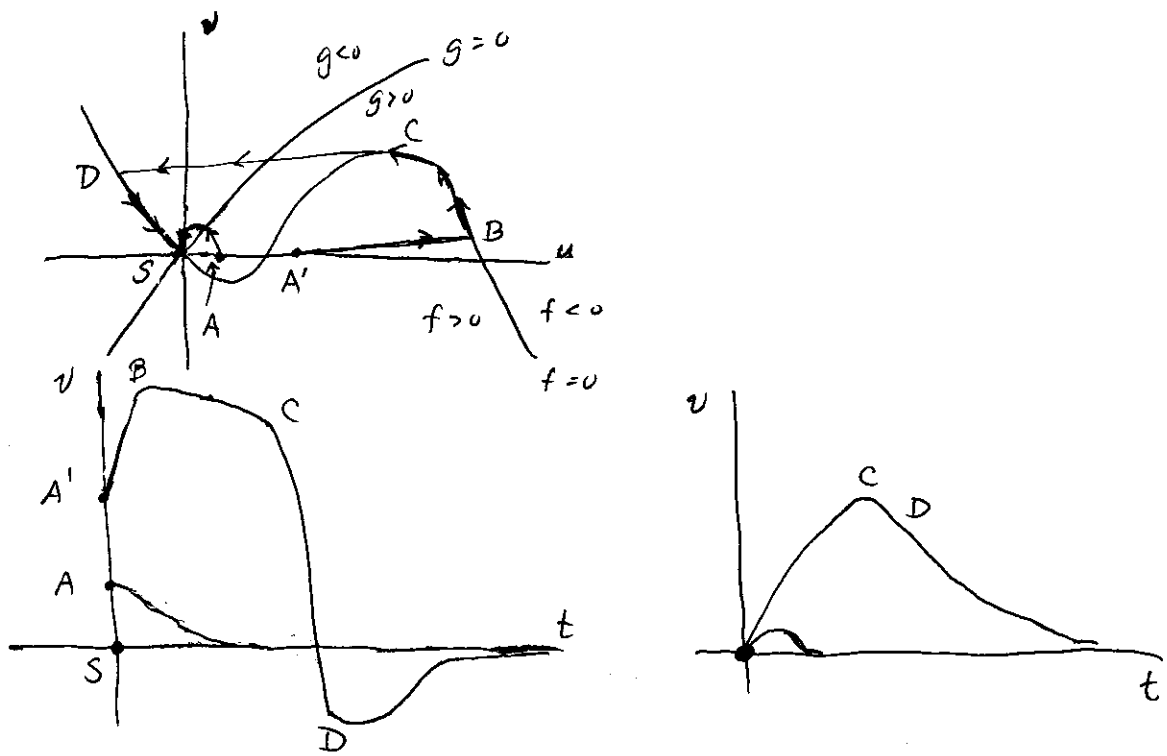
$$D = \det M = ad + bc > 0$$
$$T = \mathrm{Tr}\, M = -(a+d) < 0$$

Thus, S is always stable. It is a stable node if

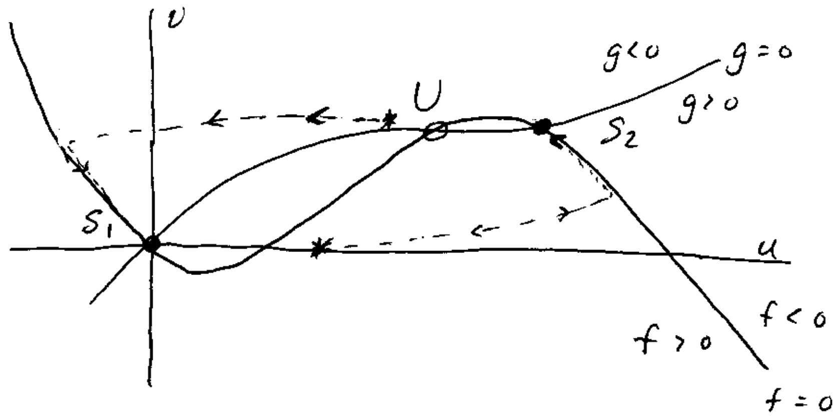
$$D < \frac{1}{4}T^2 \Rightarrow 4bc < (a-d)^2 \Rightarrow |a-d| > 2\sqrt{bc}$$

Otherwise it is a stable spiral for $|a-d| < 2\sqrt{bc}$.

Although S is stable, it is still <u>excitable</u> in that a large enough perturbation will result in a big excursion:



We also may have multiple stable states, e.g.



$S_{1,2}$: stable
U : unstable

Now a large enough perturbation from $S_{1,2}$ results in a <u>switch</u> to $S_{2,1}$. NB: often we write

$$\dot{u} = f(u,v)$$
$$\dot{v} = \epsilon\, g(u,v)$$

with $\epsilon \ll 1$. The u dynamics are fast and the v dynamics are slow.

<u>Waves in Excitable Media</u>

Let's add diffusion:

$$u_t = f(u,v) + D_{11} u_{xx} + D_{12} v_{xx}$$
$$v_t = g(u,v) + D_{21} u_{xx} + D_{22} v_{xx}$$

We consider a specific model:

$$u_t = u(a-u)(u-1) - v + Du_{xx}$$
$$v_t = bu - \gamma v$$

This is known as the FitzHugh-Nagumo model (1961-2) model nerve conduction, a tractable reduction of the seminally important Hodgkin-Huxley (1952) model. Here

$u \rightarrow$ membrane potential

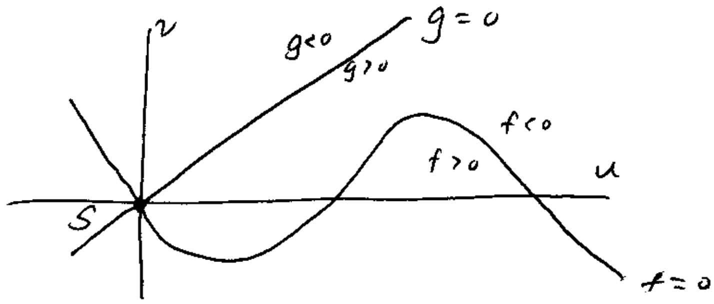
$v \rightarrow$ contributions to membrane current from Na^+, K^+ ions.

We have $0<a<1$, $b>0$, $\gamma>0$. We're interested in wave sol$^{\underline{ns}}$. Example: waves in muscle tissue, such as heart muscle.

We have

$$f(u,v) = u(a-u)(u-1) - v$$
$$g(u,v) = bu - \gamma v$$

$$u_t = f(u,v) + Du_{xx}$$
$$v_t = g(u,v)$$



Let us define $\xi \equiv x - ct$, in which case

$$Du'' + cu' + h(u) - v = 0$$
$$cv' + bu - \gamma v = 0$$

with

$$h(u) \equiv u(a-u)(u-1)$$
$$f(u,v) = h(u) - v$$

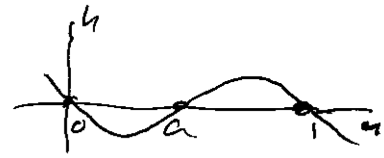
Boundary conditions on solitary pulse: $u, u', v \to 0$ as $|\xi| \to \infty$. Note we have an $N=3$ system:

$$\frac{d}{d\xi}\begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} w \\ -\frac{b}{c}u + \frac{\gamma}{c}v \\ -\frac{c}{D}w - \frac{1}{D}h(u) + \frac{1}{D}v \end{pmatrix}$$

with $w \equiv u'$.

Suppose b, γ are both small. Then a perturbation starting from $(u_0, 0, 0)$ obeys

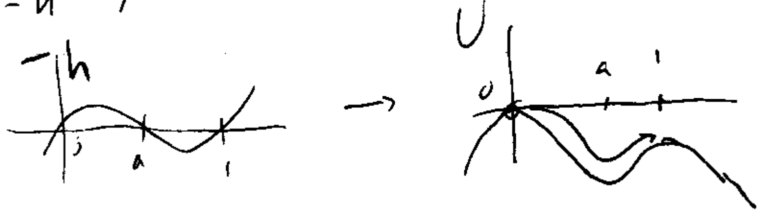
$$u_t \approx Du_{xx} + h(u)$$



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

$$Du'' + cu = -h \rightarrow m\ddot{x} + \gamma x = -U'$$

The sol$^{\underline{n}}$ is

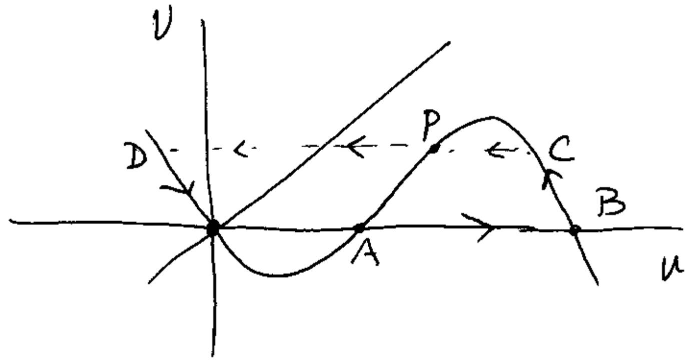


adjust γ to find unique sol$^{\underline{n}}$

$$\gamma \int dt\, \dot{x}^2 = U_i - U_f$$

$$u = u(\zeta), \quad c = \left(\tfrac{D}{2}\right)^{1/2}(1-2a)$$

So $c > 0$ requires $a < \frac{1}{2}$.



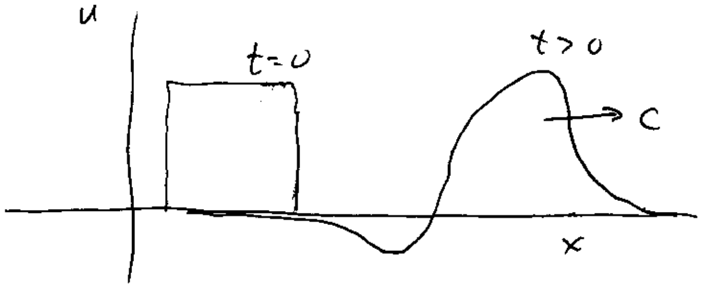
We must find C next. On CD,

$$u_t = Du_{xx} + f(u) - v_C$$

$$u = u(s), \quad u(-\infty) = u_D, \quad u(+\infty) = u_C$$

$$\rightarrow \quad \tilde{c} = (D/2)^{1/2}(u_C - 2u_P + u_D)$$

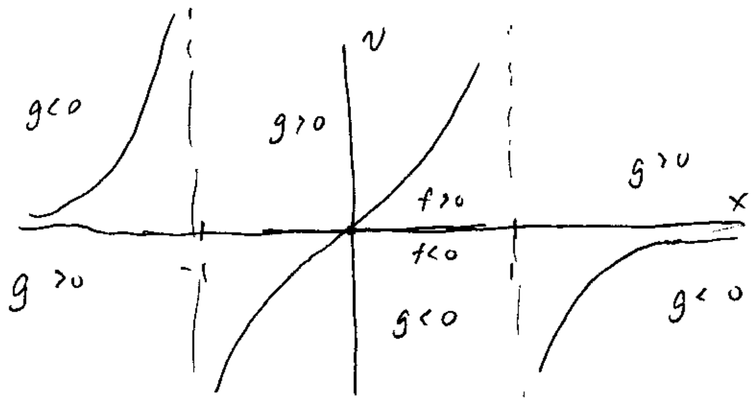
We then require $\tilde{c} = c$ to determine C.



Relaxation Oscillations

$$\ddot{x} + \mu(x^2-1)\dot{x} + x = 0$$

$$\dot{x} = v = f(x,v)$$
$$\dot{v} = -\mu(x^2-1)v - x = g(x,v)$$



$$g(x,v) = 0 \Rightarrow \quad v = -\frac{1}{\mu}\frac{x}{x^2-1}$$