Reaction-diffusion equations

in biomedical applications

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Contents

Reaction-diffusion equation

u(x,t) – depending on considered applications describes temperature or concentration distribution, the density of some populations, etc

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

$F(u)$ ← heat or mass production or reproduction rate

$\frac{\partial^2 u}{\partial x^2}$ ← mass diffusion or heat conduction or random motion of individuals

One equation or systems of equations

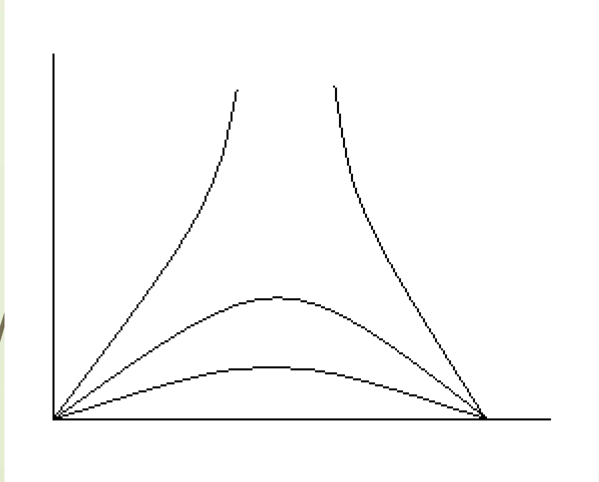
Beginning of the theory of reaction-diffusion equations

- Heat explosion (Semenov, Frank-Kamenetskii, 1930s)
- Wave propagation (Fisher, KPP, Zeldovich-Frank-Kamenetskii, 1938)
- Pattern formation (Turing, 1952)

Frank-Kamenetskii model of heat explosion

$$\frac{\partial u}{\partial t} = \Delta u + e^u$$

Temperature distribution

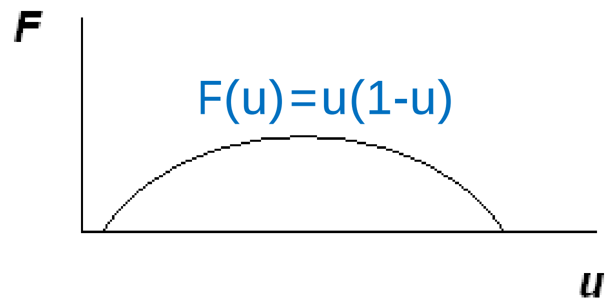


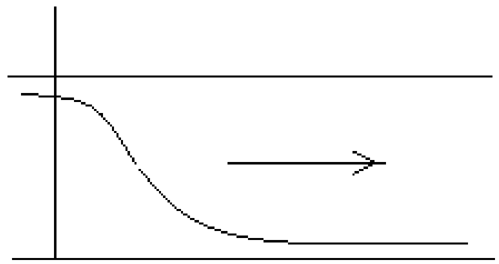
Existence of stationary solutions or blow-up (unbounded) solution?

Ammonium nitrate explosion, Beyrouth, 2020

Wave propagation (KPP-Fisher equation)

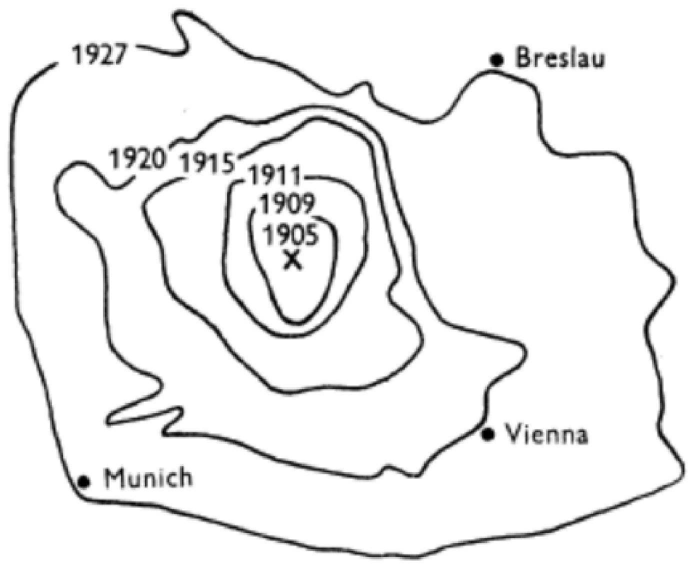
$$\frac{\partial u}{\partial t} = d\,\frac{\partial^2 u}{\partial x^2} + F(u)$$





u(x,t) = w(x-ct)

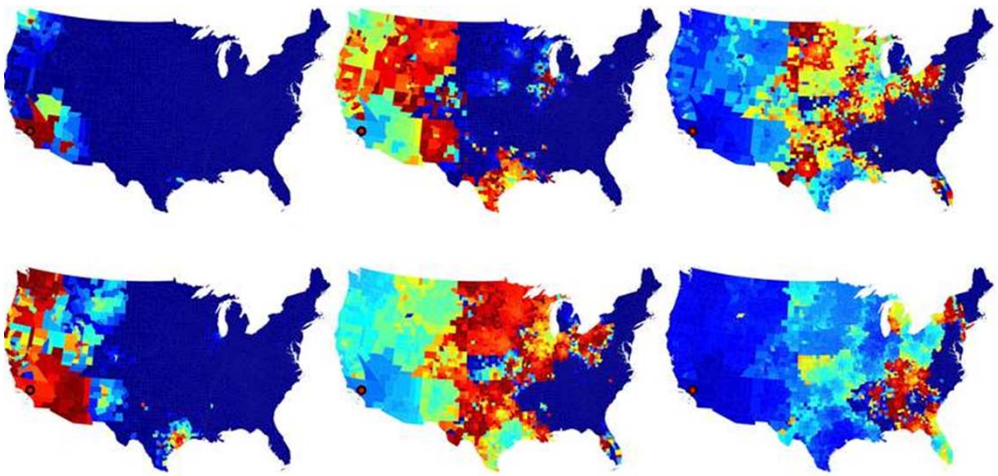
Ecological invasions



Invasion of American muskrat in Europe

Skellam, 1951

Epidemic progression

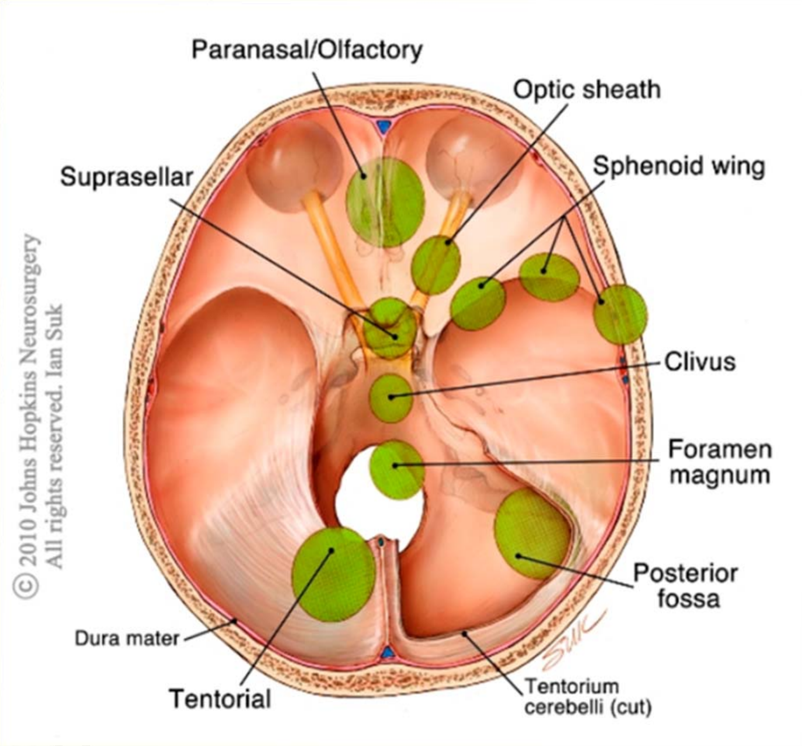


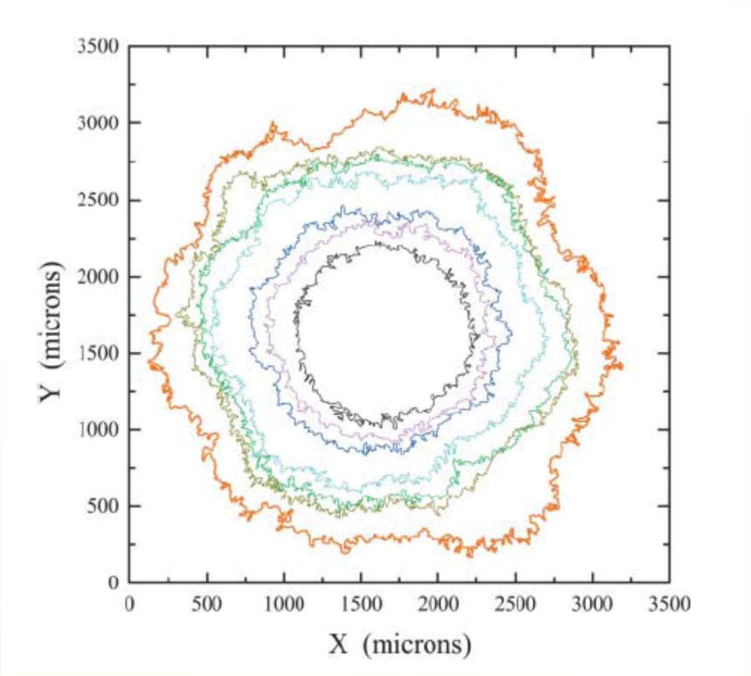
Infection spreading in the USA

Combustion engines, fires

Tumor growth

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





Excitable medium: brain, heart

Nerve impulse: Hodgkin-Huxley model

(from Keener, Sneyd)

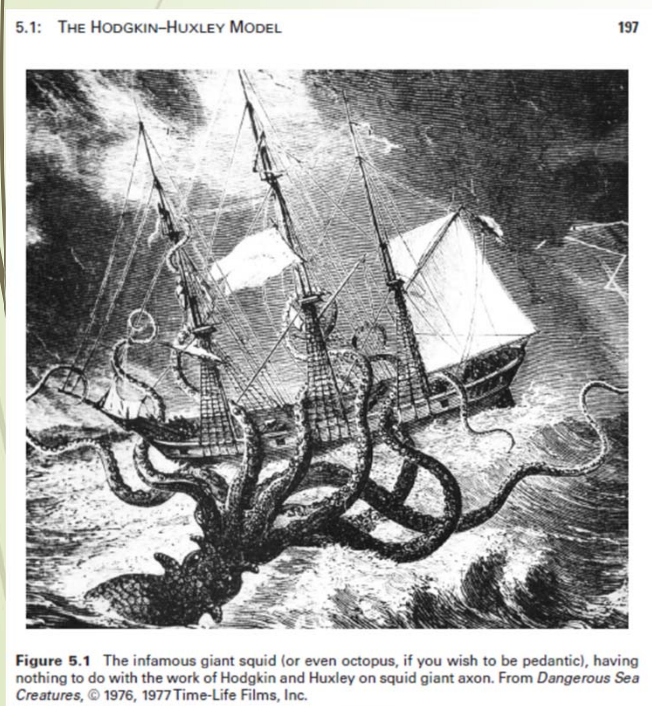
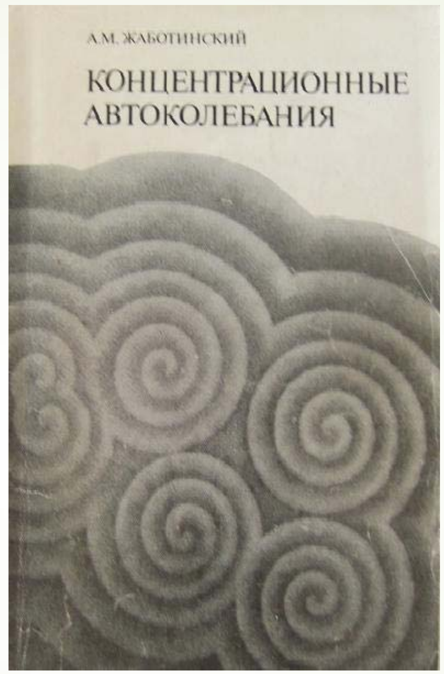

5.1: THE HODGKIN–HUXLEY MODEL 197

Figure 5.1 The infamous giant squid (or even octopus, if you wish to be pedantic), having nothing to do with the work of Hodgkin and Huxley on squid giant axon. From *Dangerous Sea Creatures*, © 1976, 1977 Time-Life Films, Inc.

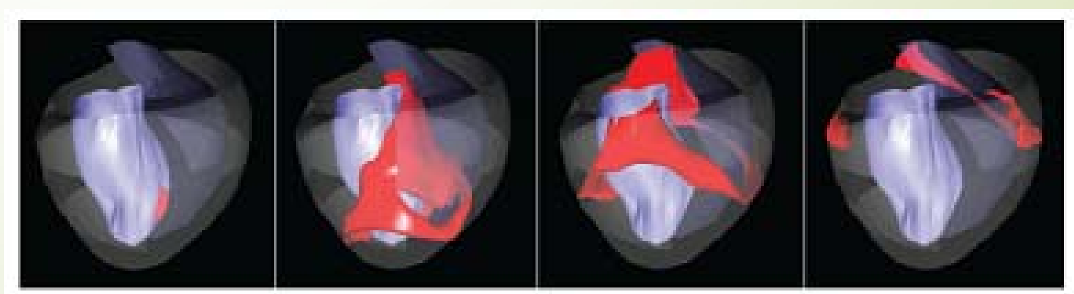


Belousov, Zhabotinskii reactions

From Zhabotinskii. Concentrational auto-oscillations. 1974.

Heart waves

(from D. Noble paper)



Pattern formation: Turing structures

$$\frac{\partial u}{\partial t} = d_u \frac{\partial^2 u}{\partial x^2} + F(u,v)$$

$$\frac{\partial v}{\partial t} = d_v \frac{\partial^2 v}{\partial x^2} + G(u,v)$$

Existence and stability of waves and pulses

Main definitions

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

Travelling wave solution:

$$u(x,t) = w(x - ct)$$

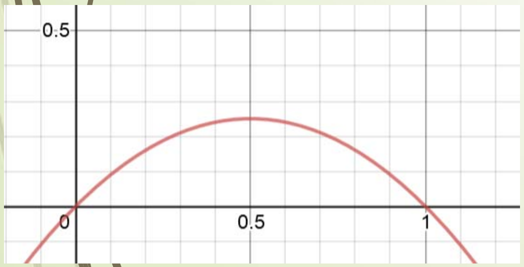
c – wave speed – unknown constant

satisfies the problem:

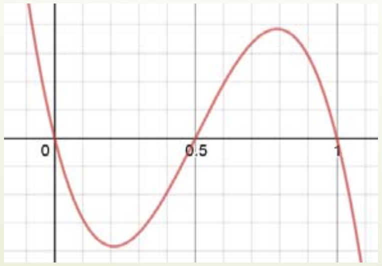
$$w'' + cw' + F(w) = 0$$

$$w(-\infty) = 1\,,\quad w(\infty) = 0$$

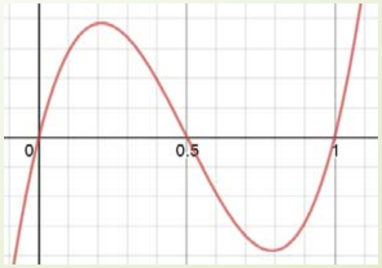
Three types of nonlinearity:



Monostable



bistable

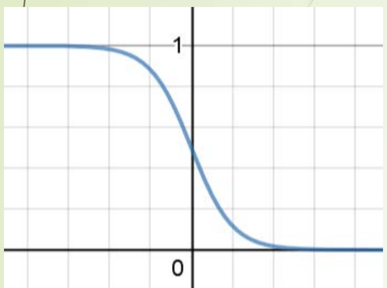


unstable

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

Wave existence: monostable case

w(x)

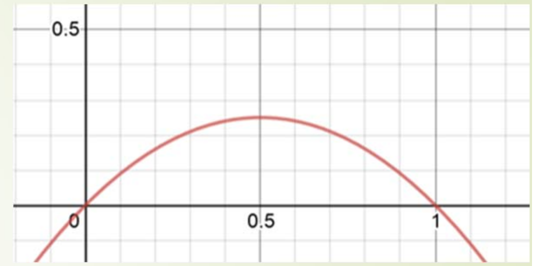


x

$$w'' + cw' + F(w) = 0$$

$$w(-\infty) = 1\,,\;\; w(\infty) = 0$$

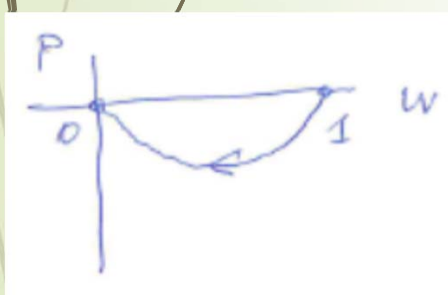
F(w)



w

First-order system:

$$w' = p\,,\quad p' = -cp - F(w)$$



We look for a trajectory connecting (1,0) and (0,0)

Stationary points

$(0,0)$ Linearized system

$$\begin{cases} w' = p \\ p' = -cp - F'(0)w \end{cases} \qquad \begin{pmatrix} w \\ p \end{pmatrix}' = A \begin{pmatrix} w \\ p \end{pmatrix}$$

$$A = \begin{pmatrix} 0 & 1 \\ -F'(0) & -c \end{pmatrix} \qquad \boxed{F'(0) > 0}$$

Eigenvalues

$$A - \lambda E = \begin{pmatrix} -\lambda & 1 \\ -F'(0) & -c-\lambda \end{pmatrix}$$

$$\det(A - \lambda E) = 0 \quad \Rightarrow$$

$$\lambda^2 + c\lambda + F'(0) = 0$$

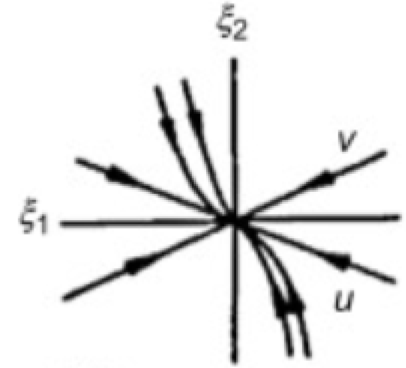
$$\lambda = -\frac{c}{2} \pm \sqrt{\frac{c^2}{4} - F'(0)}$$

$c > 2\sqrt{F'(0)}$ - stable node (equality?)

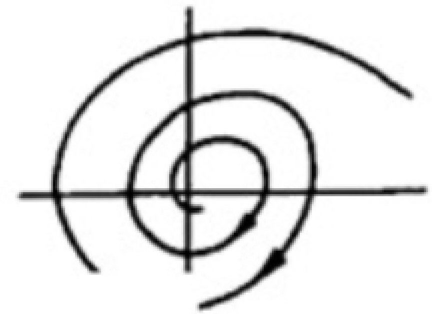
$c < -2\sqrt{F'(0)}$ - unstable node

$c^2 < 4F'(0)$ - focus

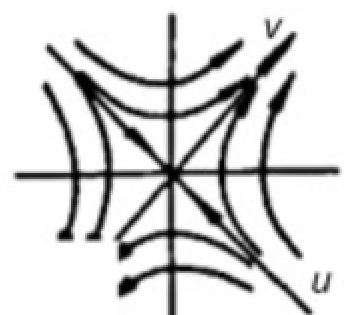
-3-



(A)



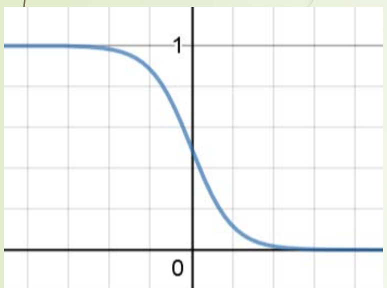
(I)



(G)

Wave existence: monostable case

w(x)

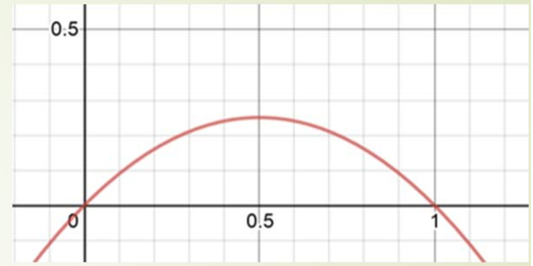


x

$$w'' + cw' + F(w) = 0$$

$$w(-\infty) = 1\,, \quad w(\infty) = 0$$

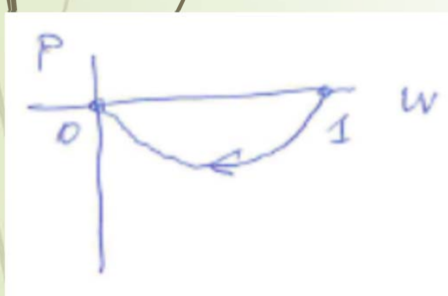
F(w)



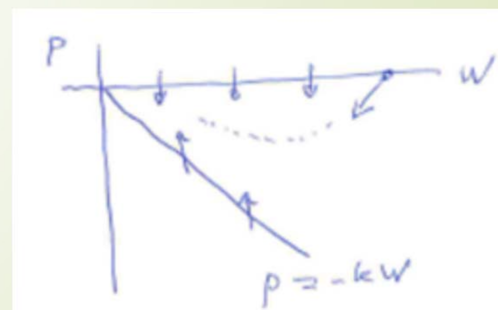
w

First-order system:

$$w' = p\,, \quad p' = -cp - F(w)$$

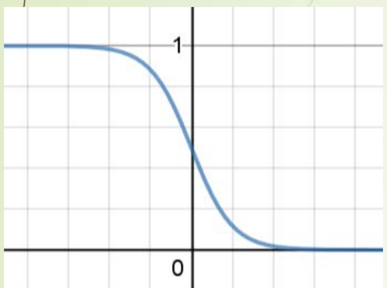


We look for a trajectory connecting (1,0) and (0,0)



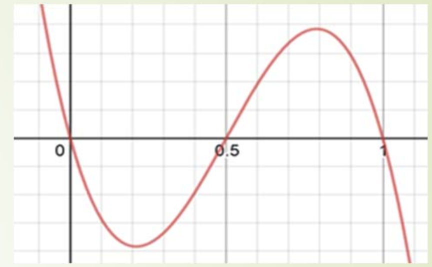
Theorem 1. Monotone waves exist for all values of the speed c greater than or equal to some minimal speed c0

Wave existence: bistable case



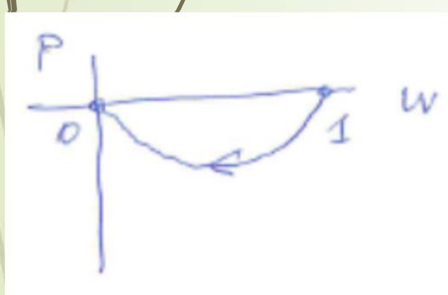
$$w'' + cw' + F(w) = 0$$

$$w(-\infty) = 1\,, \quad w(\infty) = 0$$

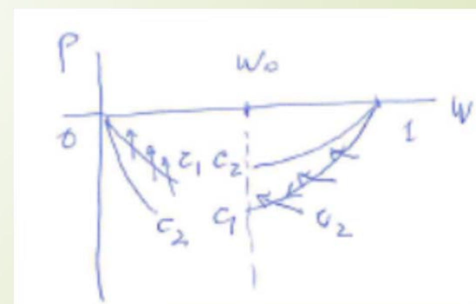


First-order system:

$$w' = p\,, \quad p' = -cp - F(w)$$



We look for a trajectory connecting (1,0) and (0,0)



Theorem 2. A monotone waves exists for a single value of speed c.

Examples

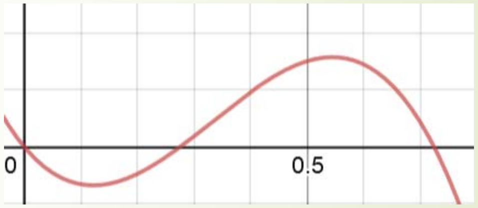
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + F(u)$$

Population dynamics

$$F(u) = au^k(1-u) - \sigma u$$

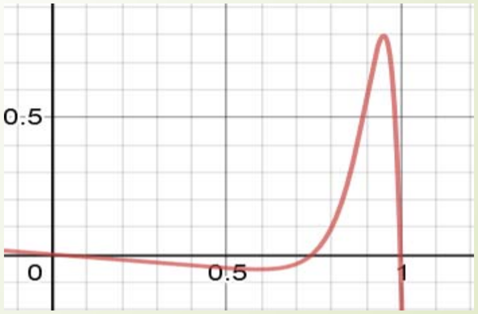
k=1

k=2



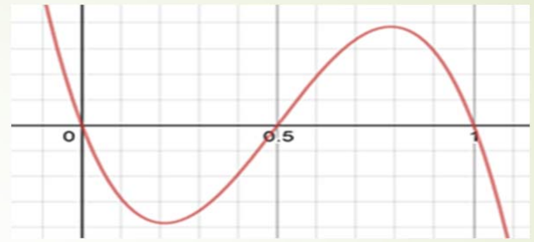
Combustion

$$F(u) = ae^{zu}(1-u) - \sigma u$$



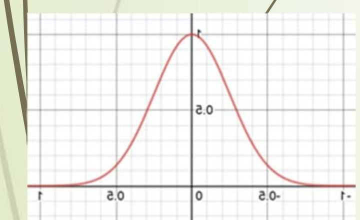
Existence of pulses

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



Pulse – positive stationary solution with 0 limits at infinity

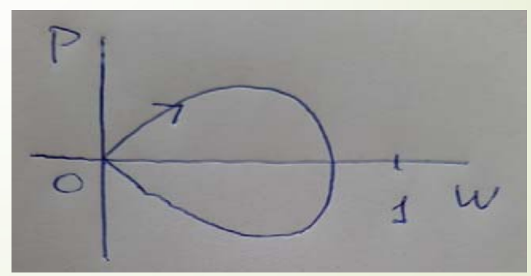
Bistable nonlinearity



$$w'' + F(w) = 0$$

$$w(\pm\infty) = 0$$

$$w' = p, \quad p' = -F(w)$$



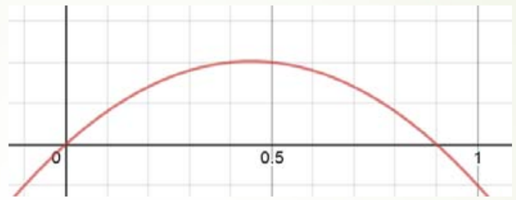
Theorem 3. Pulse exists if and only if $\int_0^1 F(u)du > 0$

Examples

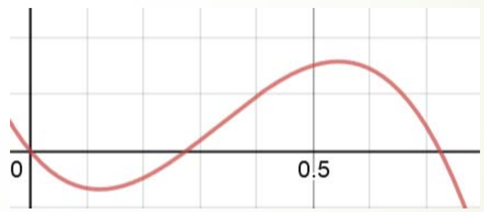
$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + F(u)$$

Local model

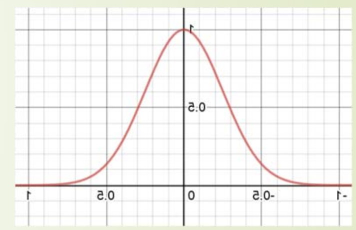
$$F(u) = au^k(1-u) - \sigma u$$



k=1 No pulse

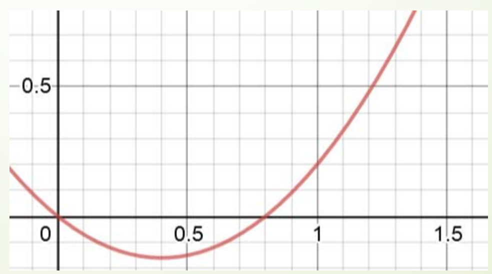


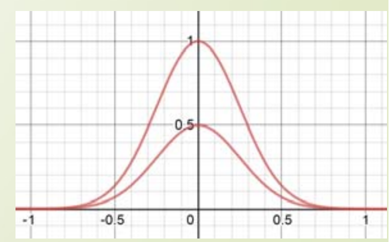
k=2



Nonlocal model

$$F(u) = au^2\left(1 - \int_{-\infty}^{\infty} u(y)dy\right) - \sigma u$$





$$r = a\left(1 - \int_{-\infty}^{\infty} u(y)dy\right)$$

$$u'' + ru^2 - \sigma u = 0$$

$$r = a\left(1 - \int_{-\infty}^{\infty} u_r(y)dy\right)$$

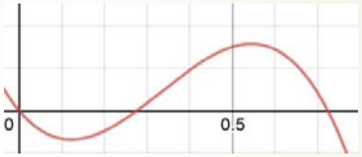
two pulses

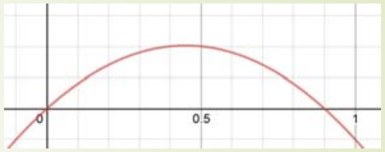
Genaralizations

- Systems of equations
- Multi-dimensional equations and systems
- Nonlocal (integrodifferential equations)
- Delay equations

Stability of waves: definitions

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





$$u(x,t) = w(x - ct)$$

$$w'' + cw' + F(w) = 0$$

$$w(-\infty) = 1\,,\quad w(\infty) = 0$$

Invariance with respect to translation: w(x+h) is a solution for any real h

Stability of waves: definitions

Wave w(x) is a solution of the equation

$$w'' + cw' + F(w) = 0$$

Linearized operator

$$Lv = v'' + cv' + F'(w(x))v$$

Existence of zero eigenvalue: L w' = 0 → the previous stability result is not applicable

Stability with shift

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

$$u(x,0) = w(x) + \phi(x)$$

Initial condition

Asymptotic stability with shift (with respect to small perturbations): for any sufficiently small perturbation, solution u(x,t) converges to the shifted wave w(x-ct+h) for some h.

Krein-Rutman theorem

Consider a linear elliptic operator in a bounded domains:

$$Lu = \Delta u + \sum_{i=1}^{n} a_i(x) \frac{\partial u}{\partial x_i} + b(x)u \qquad u|_{\partial\Omega} = 0$$

The principal eigenvalue (with the maximal real part) of the problem

$$Lu = \lambda u$$

is real, simple, and the corresponding eigenfunction is positive.
There are no other positive eigenfunctions

Remarks: valid for scalar problem and bounded domains. Can be generalized for monotone systems and unbounded domains (cf. essential spectrum)

Stability of waves (scalar equation)

Equation for the wave w(x)

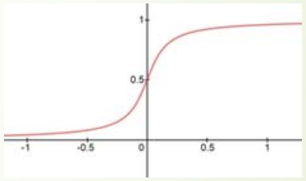
(1) $$w'' + cw' + F(w) = 0$$

$u = w'(x)$ Differentiating (1)

$$u'' + cu' + F'(w(x))u = 0$$ (2)

Linearized
operator

$$Lu = u'' + cu' + F'(w(x))u$$



u(x)=w'(x)>
0

From (2): operator L has 0 eigenvalue and the corresponding eigenfunction w'(x) is positive. Hence 0 is the eigenvalue with the maximal real part, and all other eigenvalues lie in the left half-plane.

Theorem. Monotone waves for the scalar equation are stable.

Wave speed: minimax representation

$$w'' + cw' + F(w) = 0 \quad \Rightarrow \quad c = \frac{w'' + F(w)}{-w'}$$

Test function

$$\inf_x \frac{\rho'' + F(\rho)}{-\rho'} \le c \le \sup_x \frac{\rho'' + F(\rho)}{-\rho'}$$

Minimax representation

$$c = \inf_\rho \sup_x \frac{\rho'' + F(\rho)}{-\rho'} = \sup_\rho \inf_x \frac{\rho'' + F(\rho)}{-\rho'}$$

The proof uses global asymptotic stability of waves for monotone systems

Instability of waves and pulses

Equation for the wave w(x)

(1) $$w'' + cw' + F(w) = 0$$

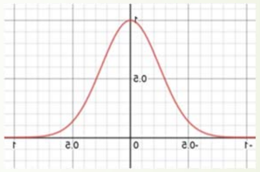
$$u = w'(x)$$

Differentiating (1)

$$u'' + cu' + F'(w(x))u = 0 \quad (2)$$

Linearized operator

$$Lu = u'' + cu' + F'(w(x))u$$



u(x)=w'(x)

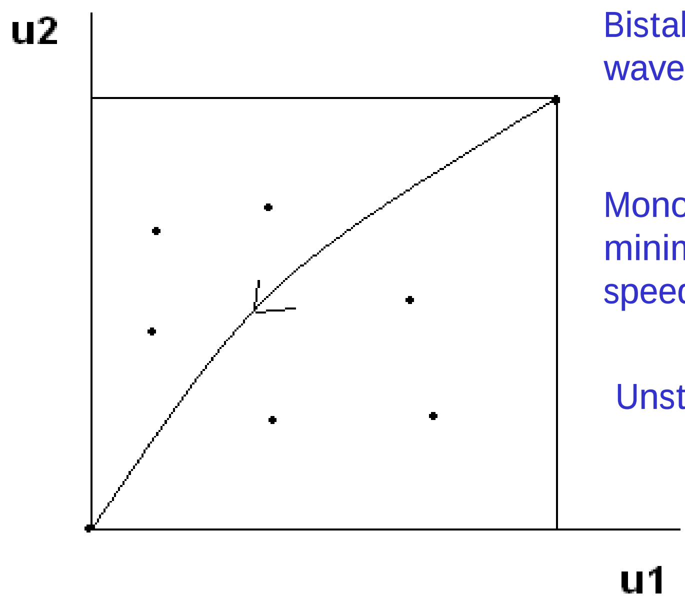
From (2): operator L has 0 eigenvalue and the corresponding eigenfunction w'(x) has variable sign. Hence 0 is not the eigenvalue with the maximal real part, and there are eigenvalues in the right half-plane.

Theorem. Non-monotone waves and pulses for the scalar equation are unstable

Reaction-diffusion systems: monotone systems

$$\frac{\partial u}{\partial t} = d\,\frac{\partial^2 u}{\partial x^2} + F(u)$$

$$\frac{\partial F_i}{\partial u_j} \geq 0, \quad i \neq j$$



Bistable: existence, uniqueness, convergence to waves, minimax representation of the speed

Monostable: existence for c>=c0, stability, minimax representation of the minimal wave speed

Unstable: non-existence