Reaction-Diffusion equations with applications

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Contents

Chapter 1

Reaction & Diffusion

1.1 Introduction

References: [5]

A reaction-diffusion equation comprises a reaction term and a diffusion term, i.e. the typical form is as follows:

$$u_t = D\Delta u + f(u)$$

$u = u(x,t)$ is a state variable and describes density/concentration of a substance, a population ... at position $x \in \Omega \subset \mathbb{R}^n$ at time t (Ω is a open set). Δ denotes the Laplace operator. So the first term on the right hand side describes the "diffusion", including D as diffusion coefficient.
The second term, $f(u)$ is a smooth function $f : \mathbb{R} \to \mathbb{R}$ and describes processes with really "change" the present u, i.e. something happens to it (birth, death, chemical reaction ...), not just diffuse in the space. It is also possible, that the reaction term depends not only on u, but also on the first derivative of u, i.e. ∇u; and/or explicitly on x.
Instead of a scalar equation, one can also introduce systems of reaction diffusion equations, which are of the form

$$u_t = D\Delta u + f(x, u, \nabla u),$$

where $u(x,t) \in \mathbb{R}^m$.

In this lecture, we will deal with such reaction-diffusion equations, from both, an analytical point of view, but also learn something about the applications of such equations.

1.2 Examples for typical reactions

In this section, we consider typical reactions which may appear as "reaction" terms for the reaction-diffusion equations. When the diffusion (i.e. spatial effects) are ignored, they are ODEs,

$$\dot{u} = f(u)$$

1.2.1 Population dynamics

Often, reaction-diffusion equations are used to describe the spread of populations in space. So, we need some basics about populations dynamics. Generally, the possible stationary states (where $\dot{u} = 0$) and their stability are of interest, which correspond to population sizes which don't change over time.

Exponential growth

$$f(u) = au$$

for $a = const.$ (the growth rate).

Logistic growth

$$f(u) = au \cdot \left(1 - \frac{u}{K}\right),$$

adding a carrying capacity K as limitation of growth.

Allee effect

$$f(u) = au \left(\frac{n}{K_0} - 1\right) \left(1 - \frac{n}{K}\right)$$

The basis of this model approach is still the logistic growth, but if the population is too low, it will also die out. Such phenomena may appear due to the necessity to find a mate for reproduction, or to defence the group against predators. This leads to the additional factor $\left(\frac{n}{K_0} - 1\right)$.

The above mentioned models concern the growth of single populations. Of course, also the interaction of several populations is of interest. The prototype are interactions of two populations, which can be formulated generally as 2D ODE:

$$\begin{aligned} \dot{x} &= f(x, y) \\ \dot{y} &= g(x, y) \end{aligned}$$

There are three typical special cases for the interaction of two populations:

1.2.2 Predator-prey

A predator population y eats from a prey population x, the most famous predator prey model (Lotka Volterra) reads

$$\begin{aligned} \dot{x} &= ax - bxy \\ \dot{y} &= cxy - dy \end{aligned}$$

Modifications are possible and often necessary; e.g. a limited growth of prey for absent predators could be introduced, or other "functional responses" (how much of the prey is eaten by the predators respectively how the predators benefit from the prey), for more details see e.g. [9].

1.2.3 Competition

Here, two species compete for a common food source. Mathematically, one species reduces the carrying capacity of the other species and vice versa. The standard approach of Lotka-Volterra reads

$$\begin{aligned} \dot{x} &= a_1 x \left(1 - \frac{x + \alpha_{12} y}{K_1}\right) \\ \dot{y} &= a_2 y \left(1 - \frac{y + \alpha_{21} x}{K_2}\right) \end{aligned}$$

1.2.4 Symbiosis

In this case, the two species benefit from each other. In some sense, it is the opposite of the competition model above: each species increases the carrying capacity of the other species.

$$\begin{aligned} \dot{x} &= a_1 x \left(1 - \frac{x - \alpha_{12} y}{K_1}\right) \\ \dot{y} &= a_2 y \left(1 - \frac{y - \alpha_{21} x}{K_2}\right) \end{aligned}$$

Of course, there are many more possibilities for such models, these are just rough basic ideas!

For more details of the modelling of population growth see e.g. [9].

1.2.5 Chemical reactions

References: [3, 6]

In many applications (bio)chemical reactions are considered, here we just collect a few very basic ideas how to translate such reactions into ODEs.

Law of mass action

We consider a very simple irreversible reaction:

$$A + B \xrightarrow{k} C,$$

k is the so-called reaction rate.
Assumption: The change of product in time corresponds to the number of collisions between molecules A and B, multiplied by the probability that indeed a reaction happens in case of collision (e.g. there is enough kinetic energy available to initialise the reaction). Let $a = [A]$, $b = [B]$, $c = [C]$ be the concentrations of A, B and C. The term $r_1 ab\Delta t$ approximates the number of collisions in Δt. For the above mentioned probability we choose a constant r_2, so the change of c in time can be described by

$$\Delta c = abk\Delta t,$$

where $k = r_1 r_2$, furthermore ($\Delta t \to 0$)

$$\frac{dc}{dt} = \dot{c}(t) = kab,$$

the so-called Law of mass action. (This is a mathematical model, not a "law")
Remark that reaction rates and concentrations should remain nonnegative!

Reversible reactions

Now we consider a reversible reaction,

$$A + B \underset{k_-}{\overset{k_+}{\rightleftharpoons}} C,$$

with the reaction rates k_+ and k_-. Assume that the split-up of C is proportional to c. The corresponding ODE system reads:

$$\begin{aligned} \frac{dc}{dt} &= k_+ ab - k_- c \\ \frac{da}{dt} &= k_- c - k_+ ab \\ \frac{db}{dt} &= k_- c - k_+ ab. \end{aligned}$$

General reaction systems

As a generalisation, we consider now r chemical reactions between s species U_i (with concentrations u_i), $i = 1, \dots s$, which interact simultaneously:

$$\sum_{i=1}^{s} l_{ij} U_i \xrightarrow{k_j} \sum_{i=1}^{s} r_{ij} U_i, \qquad j = 1, \dots r.$$

l_{ij}, r_{ij} are the so-called stoichiometric coefficients; they describe loss and gain of the number of molecules U_i in reaction j; $k_j(t)$ is the corresponding reaction rate (dependency on t might appear due to change of temperature etc.). The so-called rate function,

$$g_j(t, u) = k_j(t) \prod_{n=1}^{s} (u_n)^{l_{nj}}$$

corresponds to the speed of reaction j and can be used to formulate the ODEs for the u_i, as a net result of all reactions on U_i:

$$\dot{u}_i = \sum_{j=1}^{r} (r_{ij} - l_{ij}) g_j(t, u(t)), \qquad i = 1, \dots, s,$$

or in matrix notation

$$\dot{u} = Sg(t, u(t)),$$

where $u = (u_1, \ldots, u_s)^T$, $S = (r_{ij} - l_{ij})$ the stoichiometric matrix of size $s \times r$, $g(t, u) = (g_j(t, u)) \in \mathbb{R}^r$.

Michaelis-Menten

Literature: Murray [11], a nice short introduction can be found in Wikipedia.

The enzyme kinetics was established by Leonor Michaelis and Maud Menten in 1913. Generally, enzymes can compensate fluctuating concentrations of substrate, i.e. they adapt their activity and thereby tune a steady state. This behaviour is the common one, but of course, there are also exceptions. In opposite to the kinetics of chemical reactions, in enzyme kinetics there is the phenomenon of saturation. Even for very high concentrations of the substrate, the metabolic rate cannot be increased unlimited, there is a maximum value v_{max}.
Enzymes E, in their function as biocatalytic converter, form together with their substrate S a complex ES, from which the reaction to the product performs. Shortly, this can be noted in the following way:

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} EP \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} E + P.$$

k_1 and k_{-1} are the rate constants for the association of E and S respectively the dissociation of the enzyme - substrate complex ES. k_2 and k_{-2} are the corresponding constants for the forward reaction to the product respectively the reverse reaction to the substrate. This reverse reaction does not occur under the conditions of enzyme kinetics (short after the mixing of the components E and S). Furthermore, the conversion of ES to EP is measured (not the spontaneous release of P), thus the following simplification is justified:

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \overset{k_2}{\rightarrow} E + P.$$

(There is a nice idea, how to understand that kind of kinetics by a descriptive example: S are potatoes, the cook corresponds to the enzyme E - as he has to transform the potatoes into mashed potatoes, the product P. Obviously, the cook cannot work infinitely fast with the potatoes, only up to a limit speed; he has to deal with each potato for a certain time - there he forms a complex with the potato. And there is no chance to get back potatoes from the mushed potatoes :-)).
k_2 measures the maximal velocity of reaction under saturated substrate and is also called "turnover number". The Michaelis constant, which is the concentration of substrate, where the metabolic rate assumes half of its maximum, results in

$$K_m = \frac{k_{-1}}{k_1}$$

(in the so-called Michaelis-Menten case, if $k_2 \ll k_1$), or more generally in

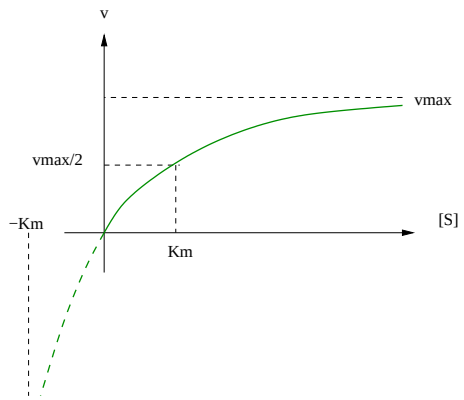
$$K_m = \frac{k_{-1} + k_2}{k_1}$$

(called Briggs Haldane situation).

The saturation function of a "Michaelis-Menten enzyme" is described by

$$v = \frac{v_{max} \cdot [S]}{K_m + [S]},$$

where $v = [\dot{P}]$, the graph looks obviously as follows:



The following variables are introduced:

s	density of S	(substrate)
e	density of E	(enzyme)
c	density of SE	(complex substrate/enzyme)
p	density of P	(product)

Then we get the following system of differential equations:

$$\begin{aligned} \dot{s} &= -k_1 se + k_{-1} c \\ \dot{e} &= -k_1 se + k_{-1} c + k_2 c \\ \dot{c} &= k_1 se - k_{-1} c - k_2 c \\ \dot{p} &= k_2 c \end{aligned}$$

with the initial conditions

$$s(0) = s_0, \quad e(0) = e_0, \quad c(0) = 0, \quad p(0) = 0.$$

Obviously, it is

$$\frac{d}{dt}(e + c) = 0,$$

thus $e + c = e_0$. Hence the system reduces to

$$\begin{aligned} \dot{s} &= -k_1 s(e_0 - c) + k_{-1} c \\ &= -k_1 s e_0 + (k_1 s + k_{-1}) c, \qquad s(0) = s_0 \\ \dot{c} &= k_1 s(e_0 - c) - k_{-1} c - k_2 c \\ &= k_1 s e_0 - (k_1 s + k_{-1} + k_2) c, \qquad c(0) = 0. \end{aligned}$$

Usually, it is assumed that c is essentially at equilibrium, thus $\frac{dc}{dt} \approx 0$, this leads to the description of c in terms of s:

$$c(t) = \frac{e_0 s(t)}{s(t) + K_m}$$

Substituting this into the equation for $\dot{s}$ yields

$$\dot{s} = -\frac{k_2 e_0 s}{s + K_m}.$$

This is called the pseudo- or quasi-steady state approximation. We consider this idea in greater detail. For that, we rescale the system (e.g. one can choose a special time scale (seconds, hours, days, ...) or a suitable scale for the concentrations (e.g. Mol or μMol or 9.87654 pMol or ...); the idea is to choose a scale which simplifies the system as much as possible. Here we choose the following rescaling:

$$\tau = (k_1 e_0) t, \qquad u(\tau) = s(t)/s_0, \qquad v(\tau) = c(t)/e_0;$$

let

$$\lambda = \frac{k_2}{k_1 s_0}, \qquad K = \frac{k_{-1} + k_2}{k_1 s_0} = \frac{K_m}{s_0}, \qquad \epsilon = \frac{e_0}{s_0}.$$

Hence

$$\begin{aligned}\frac{d}{d\tau}u(\tau) = \frac{d}{d\tau}\frac{s(t)}{s_0} &= \frac{1}{s_0}\frac{ds(t)}{dt}\frac{dt}{d\tau} \\ &= \frac{1}{s_0}\frac{1}{k_1 e_0}(-k_1 s e_0 + (k_1 s + k_{-1})c) \\ &= -\frac{s}{s_0} + \frac{1}{e_0}\frac{sc}{s_0} + \frac{k_{-1}}{k_1}\frac{c}{s_0 e_0} \\ &= -u(\tau) + u(\tau)v(\tau) + (K-\lambda)v(\tau) \\ &= -u + (u + K - \lambda)v,\end{aligned}$$

in the same way:

$$\varepsilon\frac{d}{d\tau}v(\tau) = u - (u+K)v, .$$

The initial conditions satisfy

$$u(0) = \frac{s(0)}{s_0} = 1 \quad \text{and} \quad v(0) = \frac{c(0)}{e_0} = 0.$$

Usually, there will be much less enzyme than substrate be present in the system, i.e.

$$\varepsilon = \frac{e_0}{s_0} \ll 1.$$

This means: In system

$$\begin{aligned}\dot{u} &= -u + (u + K - \lambda)v \\ \varepsilon\dot{v} &= u - (u+K)v\end{aligned}$$

there are two processes on two different time scales,

$$\begin{aligned}\dot{u} &\qquad \text{“normal”} \\ \dot{v} = \frac{1}{\varepsilon}(u - (u+K)v) &\qquad \text{“very fast” for } \varepsilon \text{ small}\end{aligned}$$

The limit $\varepsilon \to 0$ corresponds to the“pseudo steady state assumption”

$$0 = u - (u+K)v \quad \Leftrightarrow \quad v = \frac{u}{u+K}.$$

Insert this into the ODE for u:

$$\dot{u} = -u + (u + K - \lambda)\frac{u}{u+K} = -u + u - \frac{\lambda}{u+K}u = -\frac{\lambda u}{u+K}.$$

For a better understanding of the fast system, we use another time scale:

$$\hat{\tau} = (k_1 s_0)t \quad \Leftrightarrow \quad t = \frac{\hat{\tau}}{k_1 s_0}.$$

$\hat{\tau}$ is (due to $s_0 \gg e_0$) a kind of “slow motion”, i.e. a time-scale which allows to examine the short time behaviour of the fast system.
Rescaling to the time scale $\hat{\tau}$ yields

$$\begin{aligned}\frac{du}{d\hat{\tau}} &= \varepsilon(-u + (u + K - \lambda)v) \\ \frac{dv}{d\hat{\tau}} &= u - (u+K)v.\end{aligned}$$

Again, we consider the limit $\varepsilon \to 0$:

$$\begin{aligned}\frac{du}{d\hat{\tau}} &= 0 \\ \frac{dv}{d\hat{\tau}} &= u - (u+K)v\end{aligned}$$

This means: In the fast system, u doesn't change at all, so the constant value for u can be inserted into the ODE for v:

$$\frac{dv}{d\hat{\tau}} = u - (u+K)v,$$

Solution for $v(0) = v_0$:

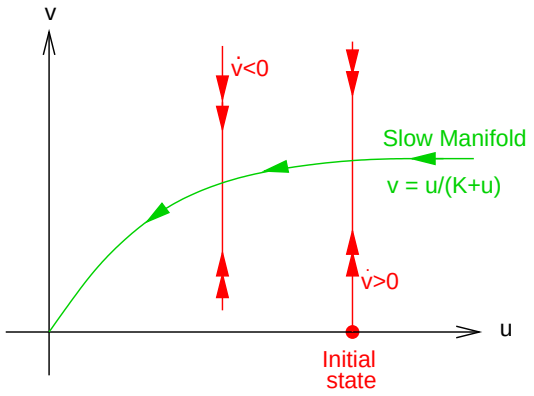
$$v(\hat{\tau}) = v_0 e^{-(u+K)\hat{\tau}} + \frac{u}{u+K}(1 - e^{-(u+K)\hat{\tau}}),$$

hence for large times

$$\lim_{\hat{\tau}\to\infty} v(\hat{\tau}) = \frac{u}{u+K}.$$

Taken together, this means:

- The formation of complexes (of enzyme and substrate) tends fast to its equilibrium, where the substrate (and also the product) nearly doesn't change.
- Then, the slow dynamics determines the behaviour: Substrate is converted (along the "slow manifold") into product, until it is used up; see also the figure:



1.3 Diffusion equation

1.3.1 Fick's law / Conservation of mass

The classical approach to the diffusion is via conservation of mass and the Fick's law.
There we start with $u(x,t) \in \mathbb{R}^3$ (as population density or substance concentration etc.) inside a container. There is a flux, denoted by $J(x,t) \in \mathbb{R}^3$, i.e. a vector which points into the general direction of movement and $|J(x,t)|$ is proportional to the amount of particles which flow in that direction per unit time.
We choose a test volume Ω with boundary Γ. If no "reactions" take place, then the only factor which influences the change of density in Ω can be a flux through Γ, i.e.

$$\frac{d}{dt}\int_\Omega u(x,t)\,dV = -\int_\Gamma J(x,t)\,dS, \tag{1.1}$$

where dV denotes the volume integral ($\mathbb{R}^n 3$), dS the surface integration ($\mathbb{R}^{3-1}$). The divergence theorem of Gauß says

$$\int_\Gamma J(x,t)\,dS = \int_\Omega \text{div } J(x,t)\,dV,$$

thus (1.1) is reformulated to

$$\int_\Omega \left(\frac{d}{dt}u + \text{div } J\right) dV = 0.$$

Since this equation is satisfied for all test volumes Ω, the integral can be left out, leading to

$$\frac{d}{dt}u + \text{div } J = 0, \tag{1.2}$$

the so-called first law of Fick (the connection between the first time-derivative of the density and the flux when assuming conservation of mass).

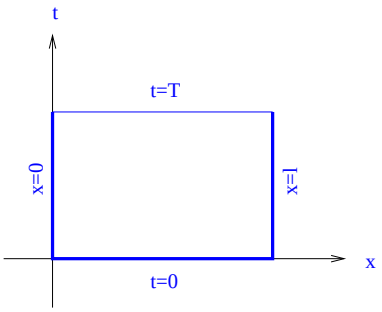


Figure 1.1: Geometrical situation for the maximum principle

Fick's second law says that the flux has the direction of the negative gradient (of the particle distribution), i.e.

$$J = -D\nabla u. \tag{1.3}$$

Inserting (1.3) into (1.2) yields the diffusion equation:

$$u_t = D\Delta u,$$

(also called heat equation).

1.3.2 (Weak) Maximum principle

Reference: [16]

As a simple example, we consider the 1D diffusion equation,

$$u_t = Du_{xx}.$$

A famous property of the diffusion equation is the so-called maximum principle:

Proposition 1 ((Weak) maximum principle for the diffusion equation) *Let $u(x,t)$ satisfy the diffusion equation in a space-time rectangle $R = \{0 \le x \le l, 0 \le t \le T\}$, then the maximum value of $u(x,t)$ is assumed either on the initial line ($t = 0$) or on the boundary lines ($x = 0$ or $x = l$).*

Proof: From Analysis we know: For a maximum in the inner of the definition area, the first derivatives have to vanish, and the second derivatives have to satisfy certain inequalities, e.g. $u_{xx} \le 0$. If we knew (which is not the case), that $u_{xx} \neq 0$ at the maximum, then we have $u_{xx} < 0$ and simultaneously $u_t = 0$, i.e. $u_t \neq u_{xx}$, a contradiction. But $u_{xx} = 0$ is possible, so we need some more effort.
Let M be the maximum of $u(x,t)$ on the three boundaries $t = 0$, $x = 0$ and $t = l$ (see Fig. 1.1). Remark that a continuous function which is defined on a bounded, closed set, is bounded and assumes its maximum on this set, so M exists. We have to show that $u(x,t) \le M$ on the whole rectangle R. Let $\varepsilon > 0$ and $v(x,t) = u(x,t) + \varepsilon x^2$. (Next goal is to show that $v(x,t) \le M + \varepsilon l^2$ in R.)
Obviously, v satisfies

$$v(x,t) \le M + \varepsilon l^2 \qquad \text{for } t = 0, x = 0 \text{ and } x = l,$$

furthermore

$$v_t - Dv_{xx} = u_t - D(u + \varepsilon x^2)_{xx} = u_t - Du_{xx} - 2\varepsilon D = -2\varepsilon D < 0, \tag{1.4}$$

which corresponds to a "diffusion inequality". Assume that v assumes its maximum at a inner point (x_0, t_0), i.e. $0 < x_0 < l$ and $0 < t_0 < T$. From analysis we know that $v_t = 0$ and $v_{xx} \le 0$ in (x_0, t_0), but this is in contradiction to (1.4). So, there is no maximum possible in the interior of R.
Next assume that $v(x,t)$ has a maximum on the upper boundary of R ($t_0 = T$, $0 < x < l$). Again, $v_{xx}(x_0, t_0) \le 0$. As $v(x_0, t_0) > v(x_0, t_0 - \delta)$, we get

$$v_t(x_0, t_0) = \lim_{\delta \searrow 0} \frac{v(x_0, t_0) - v(x_0, t - \delta)}{\delta} \ge 0,$$

which contradicts (1.4).
But somewhere in R, there must be a maximum of $v(x,t)$. Thus, it has to be on the basic line or on the

boundaries of R, and $v(x,t) \leq M + \varepsilon l^2$ is valid for whole R.
Now it follows immediately that

$$u(x,t) \leq M + \varepsilon(l^2 - x^2);$$

this inequality is valid for all $\varepsilon > 0$, so we get

$$u(x,t) \leq M \qquad \text{for } (x,t) \in R.$$

□

Remark 1 *This idea can be extended to a minimum principle and shown by using the maximum principle and applying it on the function $-u(x,t)$.*

Remark 2 *There is also a strong version of the maximum principle, which says that the maximum is not assumed in the interior of the rectangle, but exclusively on the initial line or on the boundary lines, except for a constant u. We do not show the proof here.*

1.3.3 Uniqueness

An important point is to check uniqueness of solutions for a given problem. In case of the Diffusion equation, an initial condition and boundary conditions (for finite boundaries) have to be prescribed. Here, we consider the so-called Dirichlet problem for the Diffusion equation (including an inhomogeneity f), i.e.

$$\begin{aligned} u_t - Du_{xx} &= f(x,t) \qquad \text{for } 0 < x < l \text{ and } t > 0 && (1.5)\\ u(x,0) &= \phi(x) && (1.6)\\ u(0,t) &= g(t) && (1.7)\\ u(l,t) &= h(t). && (1.8) \end{aligned}$$

(we consider the theory behind later in detail)

Proposition 2 (Uniqueness of the solution) *The Dirichlet problem of the Diffusion equation (1.5)-(1.8) has at most one solution.*

Proof:
For the proof, we use the so-called "energy integral method": Assume that there are two solutions $u_1(x,t)$, $u_2(x,t)$; let $w = u_1 - u_2$. According to the definition, w satisfies:

$$\begin{aligned} w_t - Dw_{xx} &= 0 \qquad \text{for } 0 < x < l \text{ and } t > 0\\ w(x,0) &= 0 \qquad \text{(initial condition)}\\ w(0,t) = 0 \quad &\text{and} \quad w(l,t) = 0 \qquad \text{(boundary conditions)} \end{aligned}$$

Furthermore, we get

$$0 = 0 \cdot w = (w_t - Dw_{xx}) \cdot w = \left(\frac{1}{2}w^2\right)_t + (-Dw_x w)_x + Dw_x^2.$$

This equation is integrated:

$$0 = \int_0^l \left(\frac{1}{2}w^2\right)_t dx - \underbrace{[Dw_x w]_0^l}_{=0 \text{ due to bound.cond.}} + D\int_0^l w_x^2\, dx$$

The t-derivative can be taken out of the integral, thus

$$\frac{d}{dt}\int_0^l \frac{1}{2}(w(x,t))^2\, dx = -D\int_0^l (w_x(x,t))^2\, dx \leq 0.$$

This means: The integral $\int_0^l w^2\, dx$ is monotone decreasing (in t), i.e. in each case we have

$$0 \leq \int_0^l (w(x,t))^2\, dx \leq \int_0^l \underbrace{(w(x,0))^2}_{=0 \text{ due to init.cond.}} dx = 0.$$

It follows that $w(x,t) = 0$, thus $u_1 = u_2$ for all $t \geq 0$.

□

1.3.4 Fundamental solution of the Diffusion equation

Reference: [16]

In this subsection, we consider the (1D) diffusion equation on the whole x-axis, i.e. $-\infty < x < \infty$ and $t \geq 0$. Obviously, we only need an initial condition, no boundary condition; so we consider the problem

$$u_t = Du_{xx} \qquad \text{for } -\infty < x < \infty,\ t > 0, \tag{1.9}$$

$$u(x,0) = \phi(x) \tag{1.10}$$

Idea: In a first step, we solve the problem for a special function $\phi(x)$ and in a second step derive the general solution. For that purpose, we use five so-called "invariance properties" of the Diffusion equation (1.9):

(a) The *Translation* $u(x-y,t)$ of each solution $u(x,t)$ is also a solution

(b) Each *Derivative* (u_x, u_t, u_{xx} ...) of a solution is also a solution

(c) Each *Linear combination* of solutions of (1.9) is also a solution (due to the linearity of the equation)

(d) Each *Integral* of a solution is also a solution. Let $S(x,t)$ be a solution of (1.9), then also $S(x-y,t)$ and hence also

$$v(x,t) = \int_{-\infty}^{+\infty} S(x-y,t)g(y)\,dy$$

for each function $g(y)$ if the integral converges in an adequate manner.

(e) Each *Dilation* $u(\sqrt{a}x, at)$ $(a > 0)$ of a solution is also a solution, it can be proved by applying the chain rule: Let $v(x,t) = u(\sqrt{a}x, at)$, then

$$v_t = \frac{\partial(at)}{\partial t}u_t = au_t, \qquad v_x = \frac{\partial(\sqrt{a}x)}{\partial x}u_x = \sqrt{a}u_x, \qquad v_{xx} = \sqrt{a}\sqrt{a}u_{xx} = au_{xx}$$

We look for a particular solution (denoted by $Q(x,t)$) of (1.9) satisfying the special initial condition

$$Q(x,0) = \begin{cases} 1 & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases} \tag{1.11}$$

(Remark that this initial condition doesn't vary under dilation)
Q is determined in three steps:

Step 1: Due to property (e) we know that a dilation $x \to \sqrt{a}x,\ t \to at$ leaves $Q_t = DQ_{xx}$ and the initial condition (1.11) unchanged, so also $Q(x,t)$ should remain unchanged. This is only possible if the dependency of Q on x and t is of the combination $x/\sqrt{t}$: The dilation leads $\frac{x}{\sqrt{t}}$ to $\frac{\sqrt{a}x}{\sqrt{at}} = \frac{x}{\sqrt{t}}$. So we look for $Q(x,t)$ of the following form:

$$Q(x,t) = g(p) \qquad \text{for } p = \frac{x}{\sqrt{4Dt}}, \tag{1.12}$$

the function g still has to be determined. (Remark that $\sqrt{4D}$ as an additional factor will be useful later; at the moment it doesn't play a role).

Step 2: We can formulate an ODE for g, using (1.12) and (1.9):

$$\begin{aligned} Q_t &= \frac{dg}{dp}\frac{\partial p}{\partial t} = -\frac{x}{2t\sqrt{4Dt}}g'(p) \\ Q_x &= \frac{dg}{dp}\frac{\partial p}{\partial x} = \frac{1}{\sqrt{4Dt}}g'(p) \\ Q_{xx} &= \frac{dQ_x}{dp}\frac{\partial p}{\partial x} = \frac{1}{4Dt}g''(p), \end{aligned}$$

thus

$$0 = Q_t - DQ_{xx} = -\frac{x}{2t\sqrt{4Dt}}g'(p) - \frac{1}{4t}g''(p) = \frac{1}{t}\left(-\frac{p}{2}g'(p) - \frac{1}{4}g''(p)\right),$$

the ODE for g reads

$$g'' + 2pg' = 0.$$

We find $g' = c_1 \cdot e^{-\int 2p\,dp} = c_1 \cdot e^{-p^2}$ and

$$Q(x,t) = g(p) = c_1 \cdot \int e^{-p^2}\,dp + c_2.$$

Step 3: For the integral boundaries we choose

$$Q(x,t) = g(p) = c_1 \int_0^{x/\sqrt{4Dt}} e^{-p^2}\,dp + c_2,$$

which is valid for $t > 0$. Taking into account the initial condition for $Q(x,t)$, expressed as limit $t \searrow 0$, we get:

$$\begin{aligned} \text{For } x > 0: \quad 1 &= \lim_{t\searrow 0} Q(x,t) = c_1 \int_0^{\infty} e^{-p^2}\,dp + c_2 = c_1 \frac{\sqrt{\pi}}{2} + c_2 \\ \text{For } x < 0: \quad 0 &= \lim_{t\searrow 0} Q(x,t) = c_1 \int_0^{-\infty} e^{-p^2}\,dp + c_2 = -c_1 \frac{\sqrt{\pi}}{2} + c_2, \end{aligned}$$

thus $c_1 = \frac{1}{\sqrt{\pi}}$, $c_2 = \frac{1}{2}$ and

$$Q(x,t) = \frac{1}{2} + \frac{1}{\sqrt{\pi}} \int_0^{x/\sqrt{4Dt}} e^{-p^2}\,dp \qquad \text{for } t > 0.$$

This satisfies all required conditions.

Let $S = \frac{\partial Q}{\partial x}$, according to property (b) it is also a solution of (1.9). For an arbitrary (differentiable) function ϕ with $\phi(x) = 0$ for large $|y|$, we define

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\phi(y)\,dy \qquad \text{for } t > 0. \tag{1.13}$$

According to (d), u is also solution of (1.9). Using partial integration yields

$$\begin{aligned} u(x,t) &= \int_{-\infty}^{\infty} \frac{\partial Q}{\partial x}(x-y,t)\phi(y)\,dy \\ &= -\int_{-\infty}^{\infty} \frac{\partial}{\partial y}[Q(x-y,t)]\phi(y)\,dy \\ &= -\int_{-\infty}^{\infty} Q(x-y,t)\phi'(y)\,dy - \underbrace{[Q(x-y,t)\phi(y)]_{y=-\infty}^{y=+\infty}}_{=0}, \end{aligned}$$

hence

$$\begin{aligned} u(x,0) &= \int_{-\infty}^{\infty} Q(x-y,0)\phi'(y)\,dy \\ &= \int_{-\infty}^{x} \phi'(y)\,dy = \phi(x). \end{aligned}$$

So, indeed (1.13) corresponds to the desired solution formula, where

$$S = \frac{\partial Q}{\partial x} = \frac{1}{\sqrt{4\pi Dt}} e^{-x^2/4Dt} \qquad \text{for } t > 0,$$

i.e.

$$u(x,t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} e^{-(x-y)^2/4Dt}\phi(y)\,dy. \tag{1.14}$$

S is called e.g. "Fundamental solution" or "Green function".

In most cases, it is impossible to solve the integral in (1.14) explicitely, but for some special $\phi(x)$ it can be written nicely by using the so-called "error function" (well-known in statistics):

$$Erf(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-p^2}\,dp.$$

Main properties of the error function are

$$Erf(0) = 0 \qquad \text{and} \qquad \lim_{x\to\infty} Erf(x) = 1.$$

1.3.5 Including a source

Reference: [16]

Here, we look for the solution of the inhomogeneous Diffusion equation on the real axis,

$$\begin{aligned} u_t - Du_{xx} &= f(x,t) \qquad \text{for } -\infty < x < \infty,\ 0 < t < \infty & (1.15)\\ u(x,0) &= \phi(x), & (1.16)\end{aligned}$$

$\phi(x)$ describes the initial distribution, $f(x,t)$ an additional source / sink term.
To show:

$$u(x,t) = \int_{-\infty}^{\infty} S(x-y,t)\phi(y)\,dy + \int_0^t \int_{-\infty}^{\infty} S(x-y,t-s)f(y,s)\,dy\,ds \tag{1.17}$$

is solution of (1.15). How to find this formula? The idea is as follows:
For an initial value problem for an ODE

$$\frac{du}{dt} + Au(t) = f(t), \qquad A \text{ constant} \tag{1.18}$$

the variation of constant formula yields a solution of type

$$u(t) = e^{-tA} + \int_0^t e^{(s-t)A} f(s)\,ds.$$

Let $u(t) \in \mathbb{R}^n$, $\phi \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$ (i.e. (1.18) corresponds to a coupled system of n ODEs). For $f(t) = 0$ the solution reads $u(t) = S(t)\phi$, where $S(t) = e^{-tA}$. For $f(t) \neq 0$ we multiply (1.18) with an "integrating factor" $S(-t) = e^{tA}$:

$$\frac{d}{dt}[S(-t)u(t)] = S(-t)\frac{du}{dt} + S(-t)Au(t) = S(-t)f(t),$$

which is integrated from 0 to t:

$$S(-t)u(t) - \underbrace{S(0)u(0)}_{\phi} = \int_0^t S(-s)f(s)\,ds.$$

Multiplying with $S(t)$ yields

$$u(t) = \underbrace{S(t)\phi}_{Solution of homog. eq.} + \int_0^t S(t-s)f(s)\,ds.$$

This formula looks quite similar to the approach in (1.17), there is one term corresponding to the solution of the homogeneous problem and a second term which takes into account the inhomogeneity. For the solution of the inhomogeneous Diffusion equation, we use of course S as introduced for (1.14). It is called also "source operator", as it transforms each function ϕ into a new function, i.e. is an operator.

It remains to show that (1.17) is indeed solution of the PDE and the initial condition (uniqueness of the solution is guaranteed). As the term including ϕ was already examined, we choose here $\phi = 0$ to check the second term. Deriving (1.17) yields

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial}{\partial t}\int_0^t \int_{-\infty}^{\infty} S(x-y,t-s)f(y,s)\,dy\,ds \\ &= \int_0^t \int_{-\infty}^{\infty} \frac{\partial S}{\partial t}(x-y,t-s)f(y,s)\,dy\,ds + \lim_{s\to t}\int_{-\infty}^{\infty} S(x-y,t-s)f(y,s)\,dy, \end{aligned}$$

(taking into account the singularity of $S(x-y,t-s)$ for $t-s=0$. Since $S(x-y,t-s)$ satisfies the Diffusion equation, we find

$$\begin{aligned} \frac{\partial u}{\partial t} &= \int_0^t \int_{-\infty}^{\infty} D\frac{\partial^2 S}{\partial x^2}(x-y,t-s)f(y,s)\,dy\,ds + \lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} S(x-y,\varepsilon)f(y,t)\,dy. \\ &= D\frac{\partial^2}{\partial x^2}\int_0^t \int_{-\infty}^{\infty} S(x-y,t-s)f(y,s)\,dy\,ds + f(x,t) \\ &= D\frac{\partial^2 u}{\partial x^2} + f(x,t), \end{aligned}$$

which corresponds exactly to the inhomogeneous Diffusion equation.
Check of the initial condition: Letting $t \to 0$ in (1.17) yields

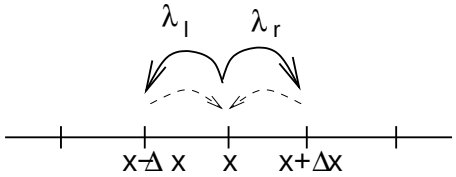
$$\lim_{t\to 0} u(x,t) = \phi(x) + \int_0^0 \ldots = \phi(x).$$

Hence, (1.17) is indeed the desired solution!

1.3.6 Random motion and the Diffusion equation

Literature: [4, 17]

The Diffusion equation can also be derived from the so-called Random walk / the "Brownian motion". Here, we consider the following 1D situation (a particle on a 1D grid):



For the Brownian motion: Per time unit τ, the particles move left or right with an average step length Δx, starting from some x. Which direction they choose, is determined randomly, there is no "connection" between the steps (thus, it is also called "uncorrelated random walk". Here, we assume equal probabilities of moving left (λ_l) or right (λ_r), i.e. $\lambda_l = \lambda_r = \frac{1}{2}$.
Let $\xi_k \in \{-\Delta x, \Delta x\}$ be the shift in the time interval $[(k-1)\Delta t, k\Delta t]$, $1 \le k \le n$ and (without loss of generality) $x = 0$ the starting point, then the complete shift after time $t = n \cdot \Delta t$ is $x_n = \sum_{k=1}^{n} \xi_k$. If r steps are made per time unit, then each step of length Δx needs $\Delta t = \frac{1}{r}$ of the time unit and n steps need $n \cdot \Delta t = \frac{n}{r}$ of the time unit. The position of the particle, x_n at time $t = n \cdot \Delta t$ can be interpreted as a random variable.
Let $u(x,t) = P(x_n = x)$ at time $t = n \cdot \Delta t$ be the probability, that the particle is at position x at time t. It can be given explicitely by the binomial distribution. The probabilities for both directions are equal. x can be displayed as $x = m \cdot \Delta x$, where $m \in \mathbb{Z}$ (i.e., it is positioned on the grid). Let n_l the number of steps to the left and n_r the number of the steps to the right, performed by the particle. Obviously,

$$n = n_l + n_r.$$

Assuming that the particle is at $m \cdot \Delta x$ after n steps, a further condition reads

$$n_r - n_l = m.$$

Taken together, it yields:

$$2n_r = n + m \quad \Leftrightarrow \quad n_r = \frac{n+m}{2}.$$

Then we can apply the probability function which belongs to the binomial distribution:

$$P(x_n = m \cdot \Delta x) = \binom{n}{n_r} \left(\frac{1}{2}\right)^{n_r} \cdot \left(\frac{1}{2}\right)^{n-n_r} = \left(\frac{1}{2}\right)^{n} \cdot \binom{n}{\frac{n+m}{2}} = \frac{1}{2^n} \cdot \binom{n}{\frac{n+m}{2}}.$$

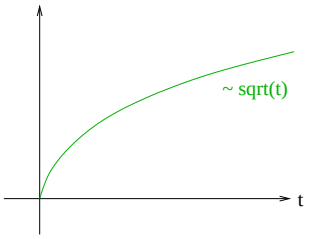
The expected value $E(x_n)$ and the variance $V(x_n)$ can be gained from the binomial distribution or determined directly:

$$\begin{aligned} E(x_n) &= E\left(\sum_{k=1}^{n} \xi_k\right) = \sum_{k=1}^{n} E(\xi_k) \\ &= \sum_{k=1}^{n} \left((-\Delta x) \cdot \underbrace{P(\xi_k = -\Delta x)}_{=\frac{1}{2}} + (\Delta x) \cdot \underbrace{P(\xi_k = \Delta x)}_{=\frac{1}{2}} \right) = 0, \end{aligned}$$

and

$$\begin{aligned} V(x_n) &= V\left(\sum_{k=1}^{n}\xi_k\right) = \sum_{k=1}^{n} V(\xi_k) \\ &= \sum_{k=1}^{n}\left((-\Delta x)^2 \cdot \underbrace{P(\xi_k = -\Delta x)}_{=\frac{1}{2}} + (\Delta x)^2 \cdot \underbrace{P(\xi_k = \Delta x)}_{=\frac{1}{2}}\right) = (\Delta x)^2 \cdot n = (\Delta x)^2 \cdot \frac{n}{t} \cdot t = (\Delta x)^2 \cdot r \cdot t. \end{aligned}$$

Thus, we find $\sqrt{V(x_n)} \sim \sqrt{t}$:



This means: The particle is always "expected" to be in the starting point (due to the "symmetry" of the choice of direction), but for a growing t, the probability is decreasing (but slower than t) that the particle is really at its starting point.

Now, we want to leave that discrete model and go to a continuous model for the Brownian motion, by letting the step size Δx tend to zero and the number of steps per time unit $r \to \infty$, in such a way that $\lim_{\Delta x \to 0, r \to \infty} (\Delta x)^2 r = 2D$, $D \neq 0$.
The number of particles in $[x, x + \Delta x]$ at time t is described by $u(x,t)\Delta x$. The corresponding discrete equation reads:

$$u(x, t + \Delta t) = u(x,t) + \lambda_r u(x - \Delta x, t) - \lambda_r u(x,t) + \lambda_l u(x + \Delta x, t) - \lambda_l u(x,t). \tag{1.19}$$

Generally, the Taylor-series expansions hold true:

$$u(x, t + \Delta t) = u(x,t) + \frac{\partial u}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial t^2}\Delta t^2 + \ldots \tag{1.20}$$

$$u(x \pm \Delta x, t) = u(x,t) \pm \frac{\partial u}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta x^2 \pm \ldots \tag{1.21}$$

Inserting (1.20) and (1.21) into (1.19) and using $\lambda_l = \lambda_r = \frac{1}{2}$ yields

$$\begin{aligned} u(x,t) + \frac{\partial u}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial t^2}\Delta t^2 + \ldots &= \frac{1}{2}\left[u(x,t) - \frac{\partial u}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta x^2 + \ldots\right] \\ &\quad + \frac{1}{2}\left[u(x,t) + \frac{\partial u}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta x^2 + \ldots\right] \\ \Leftrightarrow \quad \frac{\partial u}{\partial t}\Delta t + \frac{1}{2}\frac{\partial^2 u}{\partial t^2}\Delta t^2 + \ldots &= \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\Delta x^2 + \frac{1}{4}\frac{\partial^4 u}{\partial x^4}\Delta x^4 + \ldots \end{aligned}$$

This equation is divided through by Δt. Consider the limit $\Delta t \to 0$, $\Delta x \to 0$ in such a way that

$$\frac{(\Delta x)^2}{2\Delta t} = D = const.$$

This leads us to

$$\frac{\partial u}{\partial t} = \frac{(\Delta x)^2}{2\Delta t}\frac{\partial^2 u}{\partial x^2} = D\frac{\partial^2 u}{\partial x^2}, \tag{1.22}$$

which corresponds to the Diffusion equation. We already know: The solution of the initial value problem (1.22) with the initial condition

$$u(x, 0) = \delta(x)$$

(the Dirac δ "function") reads

$$u(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4\pi D t}}, \tag{1.23}$$

the fundamental solution.
Remark: The assumption that $\frac{(\Delta x)^2}{2\Delta t}$ tends to a finite limit $D \neq 0$, if Δx and Δt tend to zero, implicates, that the same limit yields $\frac{\Delta x}{\Delta t} \to \infty$. This means: The velocity of a particle which performs Brownian motion, is infinitely large.
This fact also follows from the solution of the initial value problem, (1.23): It is the (Gaussian) normal distribution, with expected value 0 and the variance $2Dt$. Obviously, for all $x \in \mathbb{R}$ and $t > 0$, it is $u(x,t) > 0$, thus, there is a positive probability that the particle is located in a neighbourhood of a position x, which may be located arbitrarily far away from the origin, as soon as $t > 0$. Already Einstein, who examined the connection between Brownian motion and diffusion equation first, recognised that the diffusion equation yields a valid model only for large t.

1.3.7 "Time" of Diffusion

Reference: [15]

As it could be "seen" already in the preceding section, in some sense diffusion results in a movement proportional to $\sqrt{t}$ (i.e. the standard deviation is proportional to $\sqrt{t}$). This can be considered also with a different approach, directly using the PDE.

Theorem 1 *Let u be a solution of the 1D diffusion equation*

$$u_t = Du_{xx}.$$

Assume that

$$C = \int_{-\infty}^{+\infty} u(x,t)\,dx$$

is independent of t (which corresponds to a constant "population"), and u is "small at infinity" which means that

$$\lim_{x\to\pm\infty} xu(x,t) = 0 \quad \text{and} \quad \lim_{x\to\pm\infty} x^2 \frac{\partial u}{\partial x}(x,t) = 0.$$

Let

$$\sigma^2(t) = \frac{1}{C}\int_{-\infty}^{\infty} x^2 u(x,t)\,dx,$$

then

$$\sigma^2(t) = 2Dt + \sigma^2(0)$$

for all t.
In the special case of an initial population (i.e. for $t = 0$) which is concentrated near $x = 0$ (like a δ function), then we get $\sigma^2(t) \approx 2Dt$.

Remark: $\sigma^2(t)$ is also called the ''second moment" (it is finite according to the assumptions), here we use it as a measure, how the density "spreads out".

Proof: Using the fact that u is solution of the diffusion equation, and applying integration by parts twice yields:

$$\begin{aligned}
\frac{C}{D}\frac{d\sigma^2}{dt} &= \frac{1}{D}\frac{\partial}{\partial t}\int_{-\infty}^{\infty} x^2 u\,dx \\
&= \frac{1}{D}\int_{-\infty}^{\infty} x^2 \frac{\partial u}{\partial t}\,dx \\
&= \int_{-\infty}^{\infty} x^2 \frac{\partial^2 u}{\partial x^2}\,dx \\
&= \underbrace{\left[x^2\frac{\partial u}{\partial x}\right]_{-\infty}^{+\infty}}_{=0} - \int_{-\infty}^{+\infty} 2x\frac{\partial u}{\partial x}\,dx \\
&= \underbrace{-\left[2xu\right]_{-\infty}^{+\infty}}_{=0} + \int_{-\infty}^{\infty} 2u\,dx \\
&= 2\int_{-\infty}^{\infty} u(x,t)\,dx = 2C,
\end{aligned}$$

thus

$$\frac{d\sigma^2(t)}{dt} = 2D.$$

By integration we get easily

$$\sigma^2(t) = 2Dt + \sigma^2(0),$$

as stated in the theorem.
Last, we consider the special case that the particles start in a small interval around $x = 0$, e.g. such that $u(x, 0) = 0$ for all $|x| > \varepsilon$. Then we get automatically

$$\int_{-\infty}^{\infty} x^2 u(x,0)\,dx = \int_{-\varepsilon}^{\varepsilon} x^2 u(x,0)\,dx \le \varepsilon^2 \int_{-\varepsilon}^{\varepsilon} u(x,0)\,dx = \varepsilon^2 C,$$

thus $\sigma^2(0) = \varepsilon^2 \approx 0$.

□

Chapter 2

Mathematical basics / Overview

2.1 Some necessary basics from ODE theory

Reference: [1]

As some methods / approaches for the reaction-diffusion equations (e.g. the travelling wave solutions or time-independent solutions in 1D for the space) satisfy systems of ODEs, we consider here a few details (without proofs), which may be not so well-known.

For existence and uniqueness, the most prominent theorem is the one of Picard-Lindelöf which guarantees local existence and uniqueness of a solution for $\dot{u} = f(u,t)$, where f_i are Lipschitz continuous.

Considering linear autonomous ODE systems $\dot{u} = Au$ is "easy" - the unique equilibrium 0 (if A is regular) is stable if $Re(\lambda) \leq 0$ (for all eigenvalues λ of A) with the additional condition that λ has to be a simple eigenvalue if $Re(\lambda) = 0$; it is asymptotically stable (i.e. the solutions really tend to the equilibrium, not only stay "nearby") if $Re(\lambda) < 0$ for all eigenvalues λ. Solutions can be formulated by using a fundamental system of linearly independent solutions.

For nonlinear ODE systems,

$$\dot{u} = f(u) = Au + N(u),$$

where A is a matrix and $N(u) = o(u)$ for $u \to 0$ (which means that $|N(U)|/|u| \to 0$ for $|u| \to 0$). Practically, A corresponds to the Jacobian matrix and $N(u)$ represents the remaining nonlinearity of the system. Of course, $f(u)$ is assumed to be sufficiently smooth for these operations.
The easiest way is to consider the so-called "linearised stability", i.e. to consider the linearised system $\dot{u} = Au$ and the corresponding eigenvalues for their sign. But only for the case that all eigenvalues λ have real part $\neq 0$, the stability of the linearised system can be guaranteed to correspond to that of the nonlinear system (Theorem of Hartman-Grobman). So, for some cases other methods are needed. One well-known method is to use a so-called Lyapunov function. It is defined as follows:

Definition 1 (Lyapunov function) *A function $V : \mathbb{R}^m \to \mathbb{R}$ is called positive definite if*

(a) $V(0) = 0$

(b) $V > 0$ everywhere else in an open region $\Omega \subset \mathbb{R}^m$ containing 0.

The function $V(u) = V(u(t))$ for any solution $u = u(t)$ of $\dot{u} = f(u)$ is a function of t, its derivative is (for a sufficiently smooth V) defined by

$$\frac{dV}{dt} = \dot{V} = \sum_{i=1}^{m} \frac{\partial V}{\partial u_i} \dot{u}_i = \sum_{i=1}^{m} \frac{\partial V}{\partial u_i} f_i(u)$$

If $V : \mathbb{R}^m \to \mathbb{R}$ is a function with continuous derivatives, is positive definite and $\frac{dV}{dt} \leq 0$ on Ω for any solution u of $\dot{u} = f(u)$ is called Lyapunov function for the system $\dot{u} = f(u)$.

The usefulness of the Lyapunov function is provided by the following two theorems:

Theorem 2 (Lyapunov; Stability) *If a Lyapunov function exists for $\dot{u} = f(u)$ with $f(0) = 0$, then the equilibrium at 0 is stable.*

It is even possible to proof asymptotic stability by using a Lyapunov function:

Theorem 3 (Lyapunov; Asymptotic stability) *If a Lyapunov function exists for* $\dot{u} = f(u)$ *with* $f(0) = 0$ *and* $-\frac{dV}{dt}$ *is positive definite, then the equilibrium at* 0 *is asymptotically stable.*

Often, one is interested in the asymptotic behaviour ($t \to \infty$) of solutions. Remark, that many statements in this context are only possible for 2D systems, not for higher dimensions! So, we consider here a system like that:

$$\dot{u} = f(u, v) \tag{2.1}$$
$$\dot{v} = g(u, v). \tag{2.2}$$

For showing the existence of a periodic orbit, a useful theorem is the Theorem of Poincare-Bendixson, which can be formulated as follows:

Theorem 4 (Poincare-Bendixson) *If* (u, v) *remains bounded for* $t \to \infty$ *and doesn't tend to an equilibrium, then the trajectory tends to a periodic solution.*

Remark: There are different "types" of periodic solutions / systems with periodic solutions. If f and g are sufficiently smooth and the system has at least one periodic solution, then the system either has a complete family of periodic solutions (corresponding to closed curves $G(u, v) = const$) in the phase plane, or just a number of isolated limit cycles. From a biological point or view, only the limit cycles are relevant, because the first possibility corresponds to a conservative system and includes a "structural instability", i.e. changes the behaviour under small perturbations of the system, so it wouldn't be observable in reality. So, one is not only interested in the existence / nonexistence of periodic orbits, but even more in the existence / nonexistence of stable limit cycles, as they can be observed.

For that, invariant sets are useful, they are defined as follows:

Definition 2 (Invariant set) *Let* Ω *be a domain which is enclosed by a simple curve* $\partial\Omega$ *(in the phase plane).* Ω *is called invariant set for (2.1),(2.2), if any solution with initial conditions in* Ω *stays inside* Ω *for all* $t > 0$.

The easiest way to prove a domain to be an invariant set is the following lemma:

Lemma 1 *Let* $n(u)$ *denote the unit outward normal at* $u \in \partial\Omega$. *If*

$$f(u) \cdot n(u) < 0 \qquad \forall n(u) \in \partial\Omega,$$

then Ω *is an invariant set.*

How to use invariant sets to show existence of limit cycles? There, the following theorem helps:

Theorem 5 *Let (2.1),(2.2) have an invariant set* Ω *which includes a unique unstable equilibrium (which has to be a focus). Then* ω *contains a limit cycle.*

(This theorem can be shown easily by applying the theorem of Poincare-Bendixson).

The following two theorems deal with the non-existence of limit cycles:

Theorem 6 (Negative criterion of Bendixson-Dulac) *If div* $\begin{pmatrix} f \\ g \end{pmatrix} = \frac{\partial f}{\partial u} + \frac{\partial g}{\partial v}$ *doesn't change sign in an appropriate domain* Ω*, then no limit cycles can exist in* Ω.

(This can be shown by Stokes theorem)
For the special case of considering two-component reaction systems the following theorem is useful:

Theorem 7 (Hanusse) *A two-component reaction system which contains only bi-molecular reaction cannot show up a limit cycle solution.*

For a special type of systems, existence of limit cycles follows.

Definition 3 (Lienard system) *A system which can be written as*

$$\ddot{x} + \phi(x)\dot{x} + \psi(x) = 0$$

and $\phi(x)$ *and* $\psi(x)$ *satisfy the following conditions:*

(i) $\phi(x)$ *is even,* $\psi(x)$ *is odd,* $x\psi(x) > 0$ *for all* $x \neq 0$ *and* $\phi(0) < 0$

(ii) $\phi(x)$ *and* $\psi(x)$ *are continuous;* $\psi(x)$ *satisfies a Lipschitz condition*

(iii) $\Phi(x) = \int_0^x \phi(y)\,dy \to \pm\infty$ *for* $x \to \pm\infty$, $\Phi(x)$ *has a single positive root* $x = a$ *and is a monotonic increasing function of* x *for* $x \geq a$,

is called "Lienard system".

Theorem 8 (Lienard system) *A Lienard system has a unique stable limit cycle solution.*

2.2 Boundary conditions

Reference: [5]

If we consider a reaction diffusion equation on a bounded domain $\Omega \subset \mathbb{R}^n$, i.e. $\Omega \neq \mathbb{R}^n$, then we need, additional to the initial conditions, well-suited boundary conditions (otherwise, uniqueness cannot be guaranteed). We consider the equation

$$u_t = \Delta u + f(u) \qquad \text{for } x \in \Omega \subset \mathbb{R}^n,\ t > 0$$

with the initial conditions

$$u(x,0) = u_0(x) \qquad \text{for } x \in \Omega.$$

In general, boundary conditions have the form

$$b(x,t,u,\nabla u) = 0, \qquad \text{for } x \in \partial\Omega,\ t > 0.$$

Typical examples are:

Dirichlet boundary conditions:

$$u = b(x,t) \qquad \text{for } x \in \partial\Omega,\ t > 0,$$

where b is a prescribed function. If $b = 0$, they are called homogeneous Dirichlet boundary conditions.

Neumann boundary conditions:

$$\nabla u \cdot n = b(x,t) \qquad \text{for } x \in \partial\Omega,\ t > 0,$$

where n is the outer normal to Ω at $x \in \partial\Omega$. The homogeneous case, $b = 0$, corresponds to the "no flux condition" - no particles / individuals can leave or enter the domain Ω via the boundaries.

Robin boundary conditions: (also called "mixed boundary conditions"):

$$\alpha(x,t)u + \beta(x,t)\nabla u \cdot n = b(x,t) \qquad \text{for } x \in \partial\Omega,\ t > 0,$$

notation as above.

Some remarks:

- It is possible to combine different types of boundary conditions on separate parts of the boundary.
- Here, the boundary conditions were introduced as linear conditions in u; it is possible also to have nonlinear boundary conditions (but this makes the analysis possibly more complicated).
- For the existence of solutions of reaction-diffusion equations, the choice of properly posed boundary conditions and reasonable initial data is essential. We will see that later.

2.3 Separation of Variables

References: [15, 16]

Again we start by considering the 1D diffusion equation,

$$u_t = Du_{xx}.$$

Generally, one tries to determine solution as linear combination of certain easy-to-find solution. One often useful trick is to look for a solution of the special form

$$u(x,t) = X(x)T(t).$$

This means: The dependency on variable x and variable t can be separated (an assumption!). Remark: The capitals denote the functions, not the variables. In the following, we use prime for the derivatives with respect to t and x.
Using this approach and insert it into the diffusion equation yields

$$T'(t)X(x) = DT(t)X''(x) \qquad \Leftrightarrow \qquad D\frac{X''(x)}{X(x)} = \frac{T'(t)}{T(t)} \quad \forall t, x.$$

Let

$$\lambda := \frac{T'(0)}{T(0)}.$$

The equation holds for all t and x, thus especially for $t = 0$, so we get for all x:

$$D\frac{X''(x)}{X(x)} = \frac{T'(0)}{T(0)} = \lambda,$$

(as the left hand side does not depend on t, and in the same way the right hand side does not depend on x), concluding

$$D\frac{X''(x)}{X(x)} = \frac{T'(t)}{T(t)} = \lambda \qquad \forall t, x.$$

λ is fixed, but so far unknown.
This means: X and T satisfy an linear ODE, each (with the same λ, of course). (For simplicity, we take $D = 1$ in the following; but no problem to do the same approach for $D \neq 0$):

$$\begin{aligned} X''(x) &= \lambda X(x) \\ T'(t) &= \lambda T(t). \end{aligned}$$

The second equation can be easily solved:

$$T(t) = T(0)e^{\lambda t},$$

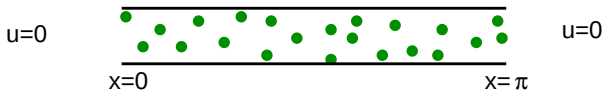
Also for the first equation, the general solution is easy to determine:

$$X(x) = ae^{+\sqrt{\lambda}x} + be^{-\sqrt{\lambda}x},$$

a, b arbitrary constants. If $\lambda < 0$, we can rewrite this solution using trigonometric functions:

$$X(x) = a\cos(\sqrt{-\lambda}x) + b\sin(\sqrt{-\lambda}x).$$

Let us consider a concrete example: Bacteria inside a thin tube (length π) which is open at both ends:



In this configuration, it is assumed that bacteria which leave the tube, are "lost" for the system, corresponding to boundary conditions

$$u(0,t) = u(\pi,t) = 0.$$

Inside the tube, we assume 1D diffusion, i.e.

$$u_t = \frac{\partial^2 u}{\partial x^2}$$

(again we use $D = 1$ for simplicity).
Remark: With these homogeneous Dirichlet boundary conditions, $u = 0$ is always a solution. We want to check if further bounded solutions $\neq 0$ are possible.
Concretely, we look for a solution with the separation of variables approach, $u(x,t) = X(x)T(t)$.
As introduced above, if a such a solution exists, then a fixed number λ exists with $X''(x) = \lambda X(x)$ and $T'(t) = \lambda T(t)$ for all x, t. Due to $T(t) = e^{\lambda t}T(0)$, it is necessary to have $\lambda \leq 0$ for a bounded solution.
$\lambda = 0$ can also be excluded, since $X''(x) = 0$ leads to $X(x) = ax + b$, but the boundary conditions would only allow for $a = b = 0$ (not a nonzero solution).
Let $k = \sqrt{\lambda}$, we know already the general form of the solution of X:

$$X(x) = a \sin kx + b \cos kx.$$

The boundary condition at $x = 0$ requires

$$X(0)T(t) = 0 \quad \text{for all } t \qquad \rightsquigarrow \qquad X(0) = 0 \qquad \rightsquigarrow \qquad b = 0.$$

So we have $X(x) = a \sin kx$ (and should have $a \neq 0$). From the boundary condition at $x = \pi$ it follows:

$$X(\pi)T(t) = 0 \quad \forall t \qquad \rightsquigarrow \qquad X(\pi) = 0 \qquad \rightsquigarrow \qquad \sin k\pi = 0.$$

This means: k must be an integer $\neq 0$.
Taken together, if there is a solution of the separated form, then it must look like

$$u(x,t) = ae^{-k^2 t} \sin kx, \qquad k \neq 0 \text{ an integer.}$$

Remark: As long as no initial conditions are given, the solution isn't unique; any linear combination of such solutions yields a solution:

$$\sum_{k \in \mathbb{Z}} a_k e^{-k^2 t} \sin kx.$$

Choosing an initial condition may shrink down the possibilities to one unique solution.
As an example, we choose as initial condition:

$$u(x,0) = 3 \sin 5x - 2 \sin 8x.$$

The presence of two frequencies (5 and 8) in the initial condition hints on that the solution could be of the form

$$u(x,t) = a_5 e^{-25t} \sin 5x + a_8 e^{-64t} \sin 8x.$$

As this solution has to satisfy the given initial condition, we can immediately determine the coefficients:

$$u(x,0) = a_5 \sin 5x + a_8 \sin 8x = 3 \sin 5x - 2 \sin 8x,$$

yielding $a_5 = 3$ and $a_8 = -2$, thus

$$u(x,t) = 3e^{-25t} \sin 5x - 2e^{-64t} \sin 8x.$$

Indeed, this is the unique solution for the given problem.

Here we had "easy" initial conditions. If they do not consist of a finite sum $\sum_k a_k \sin kx$. In the more general case, we need Fourier analysis which allows to write functions on $[0, \pi]$ as infinite sum $\sum_{k=0}^{\infty} a_k \sin kx$, where the idea works in a similar way. We do not consider this in detail here.

In the next example, we consider a reaction-diffusion equation; same situation as above, but the bacteria grow exponentially:

$$u_t = u_{xx} + \alpha u, \qquad u(0,t) = u(\pi,t) = 0.$$

The question is, under which conditions for the bacterial growth rate α the population can grow? (Remark that in the case above, without growth, the population will die out in the long term run). Easier question:

Which α allow for unbounded solutions of the separated form $u(x,t) = X(x)T(t)$?
Again, we start with the separation of variables:

$$X(x)T'(t) = X''(x)T(t) + \alpha X(x)T(t) \qquad \forall x, t,$$

a (real) λ has to exist such that

$$\frac{T'(t)}{T(t)} = \frac{X''(x)}{X(x)} + \alpha = \lambda,$$

yielding now the two coupled equations

$$\begin{aligned} T'(t) &= \lambda T(t) \\ X''(x) &= (\lambda - \alpha)X(s), \end{aligned}$$

with the boundary conditions $X(0) = X(\pi) = 0$.
If $\lambda < 0$, then $T(t) = e^{\lambda t}T(0) \to 0$ for $t \to 0$, so the solution will not be unbounded.
Thus, we choose $\lambda > 0$. Additionally we need $\lambda < \alpha$ (in order to satisfy the boundary conditions). This is shown by contradiction. Assume that $\lambda - \alpha \geq 0$. In this case, a real number μ exists, such that $\mu^2 = \lambda - \alpha$; X satisfies the equation $X'' = \mu^2 X$.
If $\mu = 0$, X becomes linear, $X = a + bx$; again, the boundary conditions imply $a = b = 0$, the solution stays bounded.
For $\mu \neq 0$ we get

$$X = ae^{\mu x} + be^{-\mu x}.$$

The boundary conditions must be satisfied, i.e. $a + b = ae^{\mu\pi} + b^{-\mu\pi} = 0$, which can be written in matrix form:

$$\begin{pmatrix} 1 & 1 \\ e^{\mu\pi} & e^{-\mu\pi} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Due to

$$det \begin{pmatrix} 1 & 1 \\ e^{\mu\pi} & e^{-\mu\pi} \end{pmatrix} = e^{-\mu\pi} - e^{\mu\pi} = e^{-\mu\pi}(1 - e^{2\mu\pi}) \neq 0,$$

the only solution is $a = b = 0$, which contradicts $X \neq 0$. Taken together, $\lambda - \alpha \geq 0$ gives a contradiction, in each case; thus $\lambda < \alpha$.
Let k be a real number with $k^2 = \alpha - \lambda$. Hence, we can derive:

$$X'' + k^2 X = 0 \qquad \rightsquigarrow \qquad X(x) = a \sin kx + b \cos kx;$$

the boundary conditions $X(0) = X(\pi) = 0$ yield $b = 0$ and $k \neq 0$ has to be an integer. Necessarily, $\alpha > 1$ is needed!
In general, the solution has the form

$$ae^{\lambda t} \sin kx = ae^{(\alpha - k^2)t} \sin kx, \qquad \text{with } a \neq 0, k \neq 0 \text{ integer.}$$

Vice versa, every function of this form (or a linear combination of it) is a solution (this has to be checked separately).
Remark: From a biological point of view, the solution only makes sense if $k = 1$, otherwise the solution contains negative values, which doesn't make sense for population densities.

2.4 Similarity solutions

Reference: [5]

Idea: By reducing a given problem (in form of a PDE) to a system which contains less independent variables, it is easier to construct solutions. Such solutions are called similarity solutions or group invariant solutions. Typical examples are so-called travelling wave solutions (for autonomous PDEs), we will consider them later in detail.

Example: We consider an equation of the form

$$G(u_t, u, u_x, u_{xx}) = 0,$$

and look for so-called plane travelling wave solutions, which means solutions of the form $u = v(z)$, where $z = x + ct$. Introducing this approach into the original equation results in an ODE for v:

$$G(cv_z, v, v_z, v_{zz}) = 0$$

(c is called the wave speed). The solution $u = v(z)$ corresponds to a surface in $\mathbb{R}^3$ (i.e. the (x, t, u)-space). Obviously, the transformation

$$x \to x - \varepsilon c, \quad t \to t + \varepsilon, \quad u \to u \tag{2.3}$$

doesn't change this surface (ε a real constant). Mathematically speaking: The solution is invariant under the group of such transformations. For fixed ε, the transformation (2.3) defines the corresponding group element. (Remark: In principle, one should check, if this group satisfies indeed the properties of a group!). Remark also, that such travelling wave solutions only make sense if the underlying PDE does not depend explicitely on x or t. If this is satisfied, the transformation (2.3) maps solution onto other solutions; but: the existence of such solutions is not trivial!
The idea of such transformations can be generalised. We consider PDEs of the form

$$G(x, t, u, u_t, u_x, \ldots) = 0. \tag{2.4}$$

Similar to above, the solution $u(x, t)$ corresponds to a surface in the (x, t, u)-space ($\mathbb{R}^3$). Now we consider a group of transformation for $\mathbb{R}^3$, dependent on one parameter $\varepsilon \in \mathbb{R}$, of the following form:

$$\begin{aligned} x &\to X(x, t, u, \varepsilon) \\ t &\to T(x, t, u, \varepsilon) \\ u &\to U(x, t, u, \varepsilon) \end{aligned} \tag{2.5}$$

such that

$$X = x, \quad T = t, \quad U = u \qquad \text{if } \varepsilon = 0.$$

If each element of the group of transformations (2.5) maps any solution of PDE (2.4) onto another solution of (2.4), then (2.5) is called symmetry group for (2.4).

Example: If we consider the 1D diffusion equation with diffusion coefficient taken to be 1,

$$u_t = u_{xx},$$

then the group of transformations

$$\begin{aligned} x &\to \varepsilon x \\ t &\to \varepsilon^2 t \\ u &\to \varepsilon^\alpha u, \end{aligned} \tag{2.6}$$

(with α fixed constant) forms a symmetry group for the diffusion equation.
How to check this? Let $U = \varepsilon^\alpha u$, $X = \varepsilon x$, $T = \varepsilon^2 t$, then one get immediately that $U_T = U_{XX}$ is true if u is a solution of the given diffusion equation.

For the more general problem (2.4): Are there any solutions which are invariant under (2.5)? Remember that such a solution corresponds to a surface in $\mathbb{R}^3$ which stays unchanged under transformations (2.5). We can formulate this condition by considering a curve

$$\{(X(x, t, u, \varepsilon), T(x, t, u, \varepsilon), U(x, t, u, \varepsilon)) : \varepsilon \in \mathbb{R}\},$$

this curve should lie in the surface whenever (x, t, u) does. Fix (x, t, u), then the set

$$\{(X(x, t, u, \varepsilon), T(x, t, u, \varepsilon), U(x, t, u, \varepsilon)) : \varepsilon \in \mathbb{R}\},$$

can be interpreted as orbit through (x, t, u).
Now we assume that there are two algebraic invariants for transformation (2.5), which means there are two functionals of the form

$$y = y(x, t, u), \quad w = w(x, t, u), \tag{2.7}$$

which are independent of ε, when the transformation (2.5) is applied - also called "leave unchanged along orbits".

(In example (2.6), one could choose $y = x^2/t$, $w = ut^{-\alpha/2}$ as such functionals)
We can specify a surface S which is invariant under the group of transformations (2.5) by a relationship between the invariants w and y - this relation corresponds to a surface in $\mathbb{R}^3$. This surface contains the whole orbits of every point in it! This means that the surface is invariant.
Vice versa, for a (given) invariant surface S, the graph of w dependent on y can be obtained; by that all the orbits which are embedded in S can be obtained, denoted by

$$w = w(y)$$

(now y is considered as new independent variable, and the variable w depends on w). How to proceed? (2.7) is assumed to be invertible, i.e. we can can write

$$\begin{aligned} u &= a(y, w, t) \\ x &= b(y, w, t) \end{aligned}$$

These expressions, and (2.7) are used to calculate the derivatives of u in terms of y, w, t and the ordinary derivatives w_y, w_{yy}.

In our example (2.6) we get:

$$u = t^{\frac{\alpha}{2}} w \qquad \text{and} \qquad x = \sqrt{yt}.$$

The derivatives read

$$\begin{aligned} u_t &= \frac{\alpha}{2} t^{\frac{\alpha}{2}-1} w + t^{\frac{\alpha}{2}} w_y y_t \\ &= \frac{\alpha}{2} t^{\frac{\alpha}{2}-1} w + t^{\frac{\alpha}{2}} w_y \frac{-x^2}{t^2} \\ &= t^{\frac{\alpha}{2}-1} \left(\frac{\alpha}{2} w - w_y y \right). \end{aligned}$$

Similarly, the x derivatives can be computed:

$$\begin{aligned} u_x &= t^{\frac{\alpha}{2}} w_y y_x \\ u_{xx} &= t^{\frac{\alpha}{2}-1} (2w_y + 4y w_{yy}) \end{aligned}$$

If u is solution of $u_t = u_{xx}$, then we get from the upper reformulations:

$$\begin{aligned} t^{\frac{\alpha}{2}-1} \left(\frac{\alpha}{2} w - w_y y \right) &= t^{\frac{\alpha}{2}-1} (2w_y + 4y w_{yy}) \\ \Leftrightarrow \qquad \frac{\alpha}{2} w - w_y y &= 2w_y + 4y w_{yy}, \end{aligned}$$

i.e. the $t^{\frac{\alpha}{2}-1}$ could be cancelled. Until now, α could be chosen arbitrarily; now we fix it to $\alpha = -1$, which yields

$$4y(w_y + \frac{w}{4})_y + 2(w_y + \frac{w}{4}) = 0.$$

It is sufficient to find a solution for $w_y + \frac{w}{4} = 0$, which reads $w = e^{-\frac{y}{4}}$. By that, we get as solution for $u_t = u_{xx}$:

$$u = t^{\frac{\alpha}{2}} w = t^{-\frac{1}{2}} e^{-\frac{x^2}{4t}}.$$

Remark: This corresponds to the already known fundamental solution!

2.5 Blow up

Also from ODEs it is known that solutions may not exist for $t \to \infty$ (global existence) but could tend to ∞ for a finite time t (thus only local existence). Similar things can happen for differential equations of the reaction-diffusion type: solutions develop a singularity. Here, two different things may happen:

- The singularity may be a point where the dependent variable tends to ∞
- The singularity may be a point where a discontinuity (or a shock) develops

If one of these phenomena occurs for finite time (and the solution cannot be continued further), this is called a "blow-up".

We consider the following example:

$$\begin{aligned} u_t &= u_{xx} - u + u^p \qquad \text{for } 0 < x < \pi,\ t > 0 && (2.8)\\ u(x,0) &= u_0(x) \geq 0 \qquad \text{for } 0 < x < \pi && (2.9)\\ u(0,t) &= u(\pi,t) = 0 \qquad \text{for } t > 0, && (2.10) \end{aligned}$$

where p is fixed.
Existence and nonnegativity can be shown (we deal with that later). We define (as auxiliary function)

$$f(t) = \int_0^\pi u(x,t) \sin x \, dx.$$

So we can multiply the PDE (2.8) by $\sin x$ and integrate it from 0 to π:

$$\begin{aligned} f_t &= \int_0^\pi u_t \sin x \, dx \\ &= \int_0^\pi u_{xx} \sin x \, dx - f + \int_0^\pi u^p \sin x \, dx \\ &= -2f + \int_0^\pi u^p \sin x \, dx. \end{aligned}$$

(Remark: We used integration in parts for this reformulation:

$$\begin{aligned} \int_0^\pi u_{xx} \sin x \, dx &= [u_x \sin x]_0^\pi - \int_0^\pi u_x \cos x \, dx \\ &= 0 - \underbrace{[u \cos x]_0^\pi}_{u(\pi,t)-u(0,t)=0,\ \text{cf. boundary cond.}} - \int_0^\pi u \sin x \, dx \\ &= -f) \end{aligned}$$

Hölder's inequality says: For $p > 1$ it holds

$$\int_a^b |gh| \, dx \leq \left(\int_a^b |g|^p \, dx \right)^{\frac{1}{p}} \left(\int_a^b |h|^{\frac{p}{p-1}} \, dx \right)^{1-\frac{1}{p}}.$$

Choose $g = u \cdot (\sin x)^{\frac{1}{p}}$ and $h = (\sin x)^{1-\frac{1}{p}}$ (and the integral boundaries $a = 0$, $b = \pi$), then we get

$$\begin{aligned} \int_0^\pi u \sin x \, dx &\leq \left(\int_0^\pi u^p \sin x \, dx \right)^{1/p} \cdot \left(\int_0^\pi \left((\sin x)^{1-\frac{1}{p}} \right)^{\frac{p}{p-1}} \, dx \right)^{1-\frac{1}{p}} \\ &= \left(\int_0^\pi u^p \sin x \, dx \right)^{1/p} \cdot \left(\int_0^\pi \sin x \, dx \right)^{1-1/p}, \end{aligned}$$

which is equivalent to

$$\int_0^\pi u^p \sin x \, dx \geq \frac{f^p}{2^{p-1}}$$

and

$$f_t = -2f + \int_0^\pi u^p \sin x \, dx \geq -2f + \frac{f^p}{2^{p-1}}.$$

Consequently, if we start with an initial value satisfying

$$f(0) = \int_0^\pi u_0(x) \sin x, dx > 2^{\frac{p}{p-1}},$$

then we get

$$f_t(0) \geq -2f(0) + \frac{f(0)^p}{2^{p-1}} = f(0) \underbrace{\left(-2 + \frac{f(0)^{p-1}}{2^{p-1}} \right)}_{>0},$$

a monotonously increasing function. We can even write down explicitely the solution of $f_t = -2f + \frac{f^p}{2^{p-1}}$, for the initial condition $f(0) = f_0$:

$$f(t) = \left(2^{-p} + e^{2(p-1)t}\left(f_0^{-p+1} - 2^{-p}\right)\right)^{-\frac{1}{p-1}}.$$

The solution tends to infinity, as

$$2^{-p} + e^{2(p-1)t^*}(f_0^{-p+1} - 2^{-p}) = 0 \quad \Leftrightarrow \quad t^* = \frac{1}{2(p-1)} \ln\left(\frac{2^{-p}}{2^{-p} - f_0^{-p+1}}\right),$$

i.e. $\lim_{t\to t^*} f(t) \to \infty$, remark that $t^* < \infty$, i.e. finite time.
Due to the Cauchy-Schwartz inequality (which can be e.g. formulated by $| < x, y > | \leq \|x\| \cdot \|y\|$) we find

$$f = \int_0^\pi u \cdot \sin x \, dx \leq \|u\|_{L_2(0,\pi)} \cdot \|\sin x\|_{L_2(0,\pi)}.$$

We already know that $f \to \infty$, thus it follows directly that $\|u\|_{L_2(0,\pi)} \to \infty$, in case of $f(0) > 2^{p/(p-1)}$, i.e. we got the blow-up in finite time.

Chapter 3

Comparison principles

Reference: [13]

In this short chapter, we try to compare different solutions of initial-boundary problems in a slightly more general context than in Chapter 1 (e.g. more general parabolic differential operators).

We consider problems of the following form:

$$\begin{aligned} u_t &= D\Delta u + f(x,t,u) \qquad \text{in } G_T = \Omega \times (0,T) \\ u &= 0 \qquad \text{on } \partial\Omega \\ u(\cdot,0) &= u_0 \qquad \text{in } \Omega, \end{aligned}$$

where $\Omega \subset \mathbb{R}^n$ is assumed to be bounded.
We start by stating the strong maximum principle:

Theorem 9 (Strong maximum principle) *Let $u \in C^2(G_T)$, $c(x,t) \geq 0$ and $D\Delta u - cu - u_t \geq 0$ in G_T. Furthermore, let $u \leq M$ in G_T (with $M \geq 0$) and $u(x_0,t_0) = M$ for a $(x_0,t_0) \in G_T$. Then it holds*

$$u(x,t) = M \qquad \forall (x,t) \in G_{t_0}.$$

(This means: If the maximum is assumed in the inner of the definition area, then the solution is constant, at least until time t_0).
From this theorem, a weak maximum principle can be derived which doesn't need a nonnegative c.

Theorem 10 (Weak maximum principle) *Let $u \in C^2(G_T) \cap C(G_T)$, $c(x,t) \geq c_{min}$ and $D\Delta u - cu - u_t \geq 0$ in G_T. Furthermore, let $u \leq 0$ in $\Omega \times \{0\}$ (i.e. for the initial condition) and in $\partial\Omega \times (0,T)$ (i.e. on the boundaries). Then it holds*

$$u(x,t) \leq 0 \qquad \forall (x,t) \in G_T.$$

Proof: We introduce an auxiliary function, $v(x,t) = e^{c_{min}t}u(x,t)$. This function satisfies

$$\begin{aligned} D\Delta v - (c - c_{min})v - v_t &= e^{c_{min}t}D\Delta u - (c - c_{min})e^{c_{min}t}u - c_{min}\underbrace{e^{c_{min}t}u(x,t)}_{v} - e^{c_{min}t}u_t \\ &= e^{c_{min}t}(D\Delta u - cu - u_t) \geq 0; \end{aligned}$$

obviously $c - c_{min} \geq 0$ according to the definition of c_{min}. Then we know from Theorem 9: v can assume a positive maximum in G_T only if it is assumed also for $t = 0$ or for $x \in \partial\Omega$. But $v \leq 0$ in $\Omega \times \{0\}$ and in $\partial\Omega \times (0,T)$, thus we get $v \leq 0$ in $G_T \rightsquigarrow u \leq 0$ in G_T.

□

The next theorem allows for comparison of two solutions in G_T:

Theorem 11 (Comparison principle) *Let $u, v \in C^2(G_T)\hat{C}(\bar{G}_T)$ and*

$$D\Delta u + f(x,t,u) - u_t \leq D\Delta v + f(x,t,v) - v_t \qquad \text{in } G_T,$$

furthermore $u \geq v$ in $\Omega \times \{0\}$ and in $\partial\Omega \times (0,T)$. Then it holds

$$u(x,t) \geq v(x,t) \qquad \forall (x,t) \in G_T.$$

Proof: Let $w = v - u$. From the mean value theorem (differential form) we know:

$$f(x,t,v) - f(x,t,u) = \frac{\partial f}{\partial u}(x,t,\xi)\underbrace{(v-u)}_{=w}$$

for a ξ satisfying

$$u(x,t) \le \xi(x,t) \le v(x,t).$$

This yields:

$$D\Delta w + c(x,t)w - w_t = D\Delta v - D\Delta u + f(x,t,v) - f(x,t,u) - v_t + u_t \ge 0$$

due to the assumption, where $c(x,t) = \frac{\partial f}{\partial u}(x,t,\xi(x,t))$. Now we can apply the weak maximum principle on w which results in

$$w \le 0 \quad \text{in } G_T \quad \rightsquigarrow \quad u \ge v \quad \text{in } G_T.$$

□

From that theorem, we get immediately a statement about uniqueness for initial boundary conditions:

Corollary 1 *Let $u_1, u_2 \in C^2(G_T) \cap C(\bar{G}_T)$ solutions of the reaction diffusion equation*

$$u_t = D\Delta u + f(x,t,u),$$

with $u_1 = u_2$ on $\Omega \times \{0\}$ and on $\partial\Omega \times (0,t)$. Then it follows that

$$u_1 = u_2 \qquad \text{in } G_T.$$

For the application of the comparison principle, we consider an example; the diffusion equation with Allee effect as reaction term:

$$u_t = \Delta u + \underbrace{u(1-u)(u-a)}_{f(u)} \qquad \text{for } x \in \Omega, \;\; t > 0, \tag{3.1}$$

where $0 < a < 1$, a const., Ω a bounded set in $\mathbb{R}^n$; the homogeneous Dirichlet boundary condition

$$u = 0 \qquad \text{on } \partial\Omega$$

and bounded initial data

$$0 \le u(x,0) \le 1 \qquad \forall x \in \Omega.$$

(Remark that the homogeneous Dirichlet condition means: no population at the boundary; possibly all individuals which arrive at the boundary are somehow "killed")
As a simple possibility, we choose a so-called sub-solution $\underline{u}(x,t)$ and a super-solution $\bar{u}(x,t)$:

$$\begin{aligned} \underline{u} &= 0 \\ \bar{u} &= 1 \end{aligned}$$

(both are independent of x), obviously both, $\underline{u}$ and $\bar{u}$ are solutions of (3.1), so we have

$$\begin{aligned} D\Delta\underline{u} + f(\underline{u}) - \underline{u}_t &\ge D\Delta u + f(u) - u_t \\ D\Delta u + f(u) - u_t &\ge D\Delta\bar{u} + f(\bar{u}) - \bar{u}_t \end{aligned}$$

and

$$\begin{aligned} u &\ge \underline{u} \qquad \text{in } \Omega \times \{0\} \text{ and } \partial\Omega \times (0,T) \\ \bar{u} &\ge u \qquad \text{in } \Omega \times \{0\} \text{ and } \partial\Omega \times (0,T), \end{aligned}$$

i.e. if a solution of (3.1) exists, then the comparison principle yields $0 \le u(x,t) \le 1$.
We can even say more: If $0 \le u(x,0) < a \;\forall x \in \Omega$, we can compare $u(x,t)$ with $s(t)$ (independent of x), where

$$s_t = s(1-s)(s-a)$$

with initial value $s(0) = \max_{x\in\Omega} u(x,0)$. Obviously s satisfies (3.1), the required comparison conditions, and it is $s(t) \to 0$ for $t \to \infty$, if $s(0) < a$, so the comparison principle yields $u \to 0$ for $t \to \infty$ (faster than $s(t)$).

Chapter 4

Existence and uniqueness

Reference: [13]

We consider the simple example (with homogeneous Neumann boundary conditions)

$$\begin{aligned} u_t &= \Delta u + f(u,t) \qquad \text{in } \Omega \times (0,\infty) \\ \frac{\partial u}{\partial \nu} &= 0 \qquad \text{for } x \in \partial\Omega. \end{aligned} \tag{4.1}$$

Obviously, each solution of the ODE $v' = f(v,t)$ is also solution (spatially independent) of equation (4.1). For ODEs, we know already that some conditions for f are necessary to guarantee existence and uniqueness of solutions. So, also for reaction-diffusion equations, conditions on f can be expected. Local existence (for small time intervals) is influenced by smoothness of f, whereas global existence is more influenced by the growth behaviour of f as function of u.

4.1 Problem formulation

Here, we consider initial boundary value problems for systems of reaction-diffusion equations,

$$u_t = D\Delta u + f(t,x,u,\nabla u), \qquad \text{for } x \in \Omega,\ t > 0 \tag{4.2}$$

$$u(x,t) = 0 \qquad \text{for } x \in \partial\Omega,\ t > 0, \tag{4.3}$$

$$u(x,t) = u_0(x) \qquad \text{for } x \in \Omega, \tag{4.4}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded domain with smooth boundary. Let $u(x,t) \in \mathbb{R}^m$ and all diffusion coefficients be positive: $D = diag(D_1, \dots, D_m)$, $D_i > 0$ for $i = 1, \dots m$. We start with $f = 0$.
From the theory of linear parabolic equations (generalisation for the diffusion equation) it is known: This problem has a unique solution for each $u_0 \in L^2(\Omega)$ (to be correct, one should write $L^2(\Omega)^m$, but the m is left out, for simplification) which can formally be written as

$$u(t) = e^{Lt} u_0,$$

the operator L is given by

$$D(L) = H^2(\Omega) \cap H_0^1(\Omega), \qquad Lu := D\Delta u.$$

Remark: Often, PDEs cannot be solved in the "classical function spaces", then so-called Sobolev spaces are needed and the concept of weak derivatives. Here, they are based on $L^2(\Omega)$. Two functions are identified if $u(x) = v(x)$ for $x \in \Omega$ except for a nullset. Via the scalar product

$$(u,v)_0 := (u,v)_{L^2} = \int_\Omega u(x)v(x)\,dx$$

$L^2(\Omega)$ becomes a Hilbert space with the norm

$$\|u\|_0 = \sqrt{(u,u)_0}.$$

The weak derivative is defined as follows: $u \in L^2(\Omega)$ has a weak derivative $v = \partial^\alpha u$ in $L^2(\Omega)$, if $v \in L_2(\Omega)$ and

$$(\phi, v)_0 = (-1)^{|\alpha|}(\partial^\alpha \phi, u)_0 \qquad \text{for all } \phi \in C_0^\infty(\Omega).$$

$\alpha = (\alpha_1, \ldots, \alpha_n) \in \mathbb{N}_0^n$ is a so-called multiindex with

$$|\alpha| = \alpha_1 + \ldots + \alpha_n,$$

e.g. it can be used as $x^\alpha = x_1^{\alpha_1} \cdot \ldots \cdot x_n^{\alpha_n}$ and $\partial^\alpha \phi = \left(\frac{\partial^{\alpha_1}}{\partial x_1^{\alpha_1}} \ldots \frac{\partial^{\alpha_n}}{\partial x_n^{\alpha_2}} \right) u$.
The idea behind is: one multiplies the weak derivative by ϕ and integrates the product by parts. The weak derivative is a generalisation of the classical derivative. If a function u is classically differentiable on a bounded domain $\Omega \subset \mathbb{R}^n$, then the classical derivative corresponds to the weak derivative.
$C_0^\infty(\Omega)$ denotes the subspace of $C^\infty(\Omega)$ which assume only in a compact subset of Ω values $\neq 0$.
If function is differentiable in the classical sense, then the weak derivative also exists and both derivatives correspond to each other.
Definition: $H^m(\Omega)$ (for $m \geq 0$ integer) denotes the set of all functions $u \in L^2(\Omega)$ which have weak derivatives $\partial^\alpha u$ for all $|\alpha| \leq m$. A scalarproduct in $H^m(\Omega)$ is defined by

$$(u, v)_m := \sum_{|\alpha| \leq m} (\partial^\alpha u, \partial^\alpha v)_0,$$

with the corresponding norm

$$\|u\|_m := \sqrt{(u, u)_m} = \sqrt{\sum_{|\alpha| \leq m} \|\partial^\alpha u\|^2_{L^2(/\Omega)}}.$$

(The letter H was chosen in honour of David Hilbert).
A proposition say: Let $\Omega \subset \mathbb{R}^n$ open with piecewise smooth boundary, $m \geq 0$. Then $C^\infty(\Omega) \cap H^m(\Omega)$ is dense in $H^m(\Omega)$. So, $H^m(\Omega)$ is the "completion" of $C^\infty(\Omega) \cap H^m(\Omega)$ for bounded Ω. This idea can be generalised for functions with zero boundary conditions $C_0^\infty(\Omega)$ and is denoted by $H_0^m(\Omega)$

Some more functional analysis, without considering all details, just to get an overview:
As the operator L has a compact symmetric inverse, there is a complete (in $L^2(\Omega)$) orthonormal system $\{\varphi_k, k = 1, 2, \ldots\}$ of eigenfunctions. Furthermore,

$$Lu = \sum_{k=1}^{\infty} \lambda_k < u, \varphi_k > \varphi_k, \qquad \text{for } u \in D(L),$$

where $0 > \lambda_1 > \lambda_2 > \ldots$ are the eigenvalues of L ($\lim_{k \to \infty} \lambda_k = -\infty$) and $< \cdot, \cdot >$ denotes the inner product (scalarproduct) in $L^2(\Omega)$.
For real functions g (with a definition area which comprises the spectrum of L), we define the operator $g(L)$ by

$$g(L)u = \sum_{k=1}^{\infty} g(\lambda_k) < u, \varphi_k > \varphi_k, \qquad \text{for } u \in D(g(L)).$$

The definition area of $g(L)$ reads

$$D(g(L)) = \left\{ u \in L^2(\Omega) : \sum_{k=1}^{\infty} g(\lambda_k)^2 < u, \varphi_k >^2 < \infty \right\}$$

(by using the so-called Parseval equality). For bounded functions, it is $D(g(L)) = L^2(\Omega)$.
The solution of the linear homogeneous initial value problem can be written as

$$u(t) = e^{Lt} u_0 = \sum_{k=1}^{\infty} e^{\lambda_k t} < u_0, \varphi_k > \varphi_k, \qquad \text{for } t \geq 0.$$

It is $u \in C([0, \infty), L^2(\Omega)) \cap C^1(0, \infty), L^2(\Omega))$, $u(t) \in D(L)$ for $t > 0$ and $du/dt(t) = Lu(t)$ for $t > 0$. The family $\{e^{Lt}, t \geq 0\}$ of bounded linear operators can be interpreted as (strongly continuous) semigroup with generator L, as the corresponding properties are satisfied:

- $e^{L(t+s)} = e^{Lt} e^{Ls}, \qquad e^{L0} = I$ (semigroup)
- $\lim_{t \to 0} e^{Lt} u = u$ (continuity)
- $\lim_{h \to 0} \frac{e^{Lh} - I}{h} u = Lu$ for $u \in D(L)$.

4.2 Abstract linear problems

Next, we consider initial value problems for so-called abstract ordinary differential equations in a Hilbert space (denoted by $\mathcal{H}$), which can be written as

$$\begin{aligned} \frac{du}{dt} &= Lu(t) + f(t), \qquad t \in (0,T], \\ u(0) &= u_0. \end{aligned} \tag{4.5}$$

We assume that the linear operator $L : D(L) \subset \mathcal{H} \to \mathcal{H}$ is defined by

$$Lu = \sum_{k=1}^{\infty} \lambda_k < u, \varphi_k > \varphi_k, \qquad u \in D(L)$$

as above, and $\{\varphi_k, k = 1, 2, \ldots\}$ forms a complete orthonormal system in $\mathcal{H}$ and it holds that

$$0 > \lambda_1 > \lambda_2 > \ldots, \qquad \lim_{k\to\infty} \lambda_k = -\infty.$$

With these assumptions, one gets the following lemma:

Lemma 2 *The definition domain $D(L)$ is dense in $\mathcal{H}$, and L is a closed operator.*

The proof is left out here; "closed linear operators" are an important class of linear operators on Banach spaces (something more general than bounded operators, but e.g. the spectrum can be defined).

In the following, the inhomogeneity f is assumed to satisfy $f \in C([0,T], \mathcal{H})$.
A classical solution is defined as follows:

Definition 4 *A classical solution $u \in C([0,T], \mathcal{H}) \cap C^1((0,T], \mathcal{H})$ of problem (4.5) must satisfy $u(t) \in D(L)$ for $t \in (0,T]$, and be solution of (4.5).*

(Remark: $u(t) \in D(L)$ means: $u \in L^2(\Omega)$ and $\sum_{k=1}^{\infty} \lambda_k^2 < u, \varphi_k >^2 < \infty$.
One idea to find such a solution is the variation of constant formula:

$$u(t) = e^{Lt}u_0 + \int_0^t e^{L(t-s)} f(s)\, ds \tag{4.6}$$

This function is called "mild solution", which is in some sense a generalisation of the concept of a solution.

Proposition 3 *There is at most one classical solution of (4.5). If it exists, then it is equal to the mild solution (4.6).*

Proof: Assume, that a classical solution u exists. Let $g(s) = e^{L(t-s)}u(s)$. By deriving this g, we get:

$$\begin{aligned} \frac{dg}{ds} &= -Le^{L(t-s)}u(s) + e^{L(t-s)}(Lu(s) + f(s)) \\ &= e^{L(t-s)} f(s). \end{aligned}$$

This equation can be integrated (for s from 0 to t) and yields

$$e^0 u(t) - e^{Lt}u(0) = g(t) - g(0) = \int_0^t \frac{dg}{ds}\, ds = \int_0^t e^{L(t-s)} f(s)\, ds$$

$$\Leftrightarrow \qquad u(t) = e^{Lt}u_0 + \int_0^t e^{L(t-s)} f(s)\, ds,$$

which corresponds exactly to (4.6).

□

We shortly mention (without proof) an auxiliary lemma which helps to show the existence of the classical solution:

Lemma 3 *For each $\delta > 0$ there exists a $c > 0$ such that*

$$\|Le^{Lt}\| \le ct^{-1}e^{(\lambda_1+\delta)t}, \qquad \text{for } t > 0.$$

We need to know how a locally Hölder continuous function is defined:

Definition 5 *A function f is called locally Hölder continuous, if for all $t \in (0, T]$ there exist $\delta, c, \alpha > 0$ such that*

$$\|f(t_1) - f(t_2)\| \le c|t_1 - t_2|^\alpha, \qquad \text{for } t_1, t_2 \in (t-\delta, t+\delta),$$

where $\|u\| = \sqrt{< u, u >}$ is the norm which is induced by the scalar product in $\mathcal{H}$.

Proposition 4 (Existence classical solution) *Let f be locally Hölder continuous in $(0, T]$. Then problem (4.5) possesses a classical solution.*

Rough idea for the proof of this proposition: It is sufficient to show that

$$\begin{aligned} v(t) &= \int_0^t e^{L(t-s)} f(s)\, ds = v_1(t) + v_2(t) \\ &= \int_0^t e^{L(t-s)}[f(s) - f(t)]\, ds + \int_0^t e^{L(t-s)} f(t)\, ds \end{aligned}$$

is a classical solution of the problem with homogeneous initial condition; for that $v(t) \in D(L)$ for $t > 0$ is needed, and $Lv(t)$ is continuous for $t > 0$. For that, Lemma 3 is useful.

4.3 Abstract semilinear problems

Here, we generalise the approaches to nonlinear problems of the following form:

$$\begin{aligned} \frac{du}{dt}(t) &= Lu(t) + f(t, u(t)), \qquad \text{for } t > 0, \\ u(0) &= u_0. \end{aligned} \tag{4.7}$$

For the operator L we take the same assumptions as in the section above.
We will need powers $(-L)^\alpha$ for $0 \le \alpha \le 1$. Introduce as new notations

$$\mathcal{H}_\alpha := D((-L)^\alpha) \qquad \text{and } \|u\|_\alpha := \|(-L)^\alpha u\|$$

Also $(-L)^\alpha$ (as L) is a closed operator; thus $\mathcal{H}_\alpha$ is a Banach space with respect to the so-called Graph norm $\|u\| + \|u\|_\alpha$. We find:

$$\begin{aligned} \|u\|^2 &= \sum_{k=1}^{\infty} < u, \varphi_k >^2 \\ &\le (-\lambda_1)^{-2\alpha} \sum_{k=1}^{\infty} (-\lambda_k)^{2\alpha} < u, \varphi_k >^2 \\ &= (-\lambda_1)^{-2\alpha} \|u\|_\alpha^2 \end{aligned}$$

(the first equality is due to Parseval's equation; due to $0 > \lambda_1 > \lambda_2 > \ldots, \lim_{k\to\infty} \lambda_k = -\infty$ it is $(-\lambda_k)^{2\alpha}/(-\lambda_1)^{2\alpha} \ge 1$)
Hence, it follows that the graph norm is equivalent to the norm $\|u\|_\alpha$ and we can use this as norm on $\mathcal{H}_\alpha$.
The next lemma provides auxiliary estimates:

Lemma 4 *Let $0 \le \alpha \le 1$, then it holds*

$$\|(-L)^\alpha e^{Lt}\| \le c_\alpha t^{-\alpha}, \qquad \text{for } t > 0 \tag{4.8}$$

$$\|e^{Lt}u - u\| \le t^\alpha \|(-L)^\alpha u\|, \qquad \text{for } t \ge 0,\ u \in \mathcal{H}_\alpha. \tag{4.9}$$

Proof: For all $x \in \mathbb{R}$ it is $ex \leq e^x$, choosing $x = -\lambda_k t/\alpha$, we get

$$\begin{aligned} & -e\lambda_k t/\alpha && \leq && e^{-\frac{\lambda_k t}{\alpha}} \\ \Leftrightarrow \quad & -e^{\frac{\lambda_k t}{\alpha}} \frac{\lambda_k t}{\alpha} e && \leq 1 \\ \Leftrightarrow \quad & -\lambda_k e^{\frac{\lambda_k t}{\alpha}} && \leq \left(\tfrac{\alpha}{e}\right) \tfrac{1}{t} \\ \Leftrightarrow \quad & (-\lambda_k)^\alpha e^{\lambda_k t} && \leq && \left(\frac{\alpha}{e}\right)^\alpha t^{-\alpha}. \end{aligned}$$

Generally (definition of the operator),

$$(-L)^\alpha e^{Lt} u = \sum_{k=1}^{\infty} (-\lambda_k)^\alpha e^{\lambda_k t} < u, \varphi_k > \varphi_k,$$

by using the Parseval equation we get:

$$\begin{aligned} \|(-L)^\alpha e^{Lt} u\|^2 &= \sum_{k=1}^{\infty} |(-\lambda_k)^\alpha e^{\lambda_k t} < u, \varphi_k > \varphi_k| \\ &\leq \underbrace{(\lambda_{\hat{k}})^\alpha e 1^{\lambda_{\hat{k}} t}}_{\leq \left(\frac{\alpha}{e}\right)^\alpha t^{-\alpha}} \underbrace{\sum_{k=1}^{\infty} | < u, \varphi_k > \varphi_k|}_{\|u\|^2} \end{aligned}$$

($\lambda_{\hat{k}}$ is chosen to yield the maximum of this term), taken together

$$\|(-L)^\alpha e^{Lt}\| \leq c_\alpha t^{-\alpha}.$$

Analogously, one can show the second inequality.

□

In the next step, we formulate a condition/assumption for the nonlinearity f in (4.7) which should be sufficient for the unique solubility. Let $0 \leq \alpha < 1$ and U an open subset of $\mathcal{H}_\alpha$.

Assumption (NONLIN): For $f : [0, T) \times U \to \mathcal{H}$ let exist for each $u_0 \in U$ a neighbourhood $V \subset U$ of u_0, and $\bar{t} \leq T$, $L \geq 0$ and $0 < \vartheta \leq 1$, such that

$$\|f(t_1, u_1) - f(t_2, u_2)\| \leq L \left(|t_1 - t_2|^\vartheta + \|u_1 - u_2\|_\alpha \right) \qquad \text{for } t_1, t_2 < \bar{t},\ u_1, u_2 \in V.$$

Theorem 12 *Let assumption (NONLIN) hold. Then for each $u_0 \in U$ a $t_0 > 0$ exists, such that (4.7) has a unique classical solution $u \in C([0, t_0), \mathcal{H}) \cap C^1((0, t_0), \mathcal{H})$.*

Proof: We write the neighbourhood from (NONLIN) in the following way:

$$V = \{u \in \mathcal{H}_\alpha : \|u - u_0\|_\alpha \leq \delta\}$$

. Furthermore, let

$$B = \max_{0 \leq t \leq \bar{t}} \|f(t, u_0)\|.$$

This maximum exists as f is continuous in $[0, \bar{t}]$. Now we choose $t_0 > 0$ such that both,

$$\|e^{Lt}(-L)^\alpha u_0 - (-L)^\alpha u_0\| < \frac{\delta}{2}, \qquad \text{for } 0 \leq t < t_0$$

and

$$t_0 < \min \left\{ \bar{t}, \left(\frac{\delta(1-\alpha)}{2c_\alpha(B + \delta L)} \right)^{\frac{1}{1-\alpha}} \right\}$$

are satisfied (c_α is the constant from the lemma above). Let

$$\chi = C([0, t_0], \mathcal{H}) \quad \text{and} \quad \|x\|_\chi = \max_{0 \leq t \leq t_0} \|x(t)\| \quad \text{for } x \in \chi.$$

We define a nonlinear operator $F : \chi \to \chi$ by

$$F(x)(t) = e^{Lt}(-L)^{\alpha}u_0 + \int_0^t (-L)^{\alpha} e^{L(t-s)} f(s, (-L)^{-\alpha}x(s))ds.$$

Obviously it is $F(x)(0) = (-L)^{\alpha}u_0$ for all $x \in \chi$. We define a set S:

$$S = \{x \in \chi : x(0) = (-L)^{\alpha}u_0, \|x - (-L)^{\alpha}u_0\|_{\chi} \le \delta\}.$$

Remark: For $x \in S$ and for $t \in [0, t_0]$ it is $(-L)^{-\alpha}x(t) \in V$.
Let $x \in S$, then we get (using the lemma above and the remark; remember also $x \in S$):

$$\begin{aligned}
\|F(x)(t) - (-L)^{\alpha}u_0\| &\le \|e^{Lt}(-L)^{\alpha}u_0 - (-L)^{\alpha}u_0\| \\
&\quad + \left\| \int_0^t (-L)^{\alpha} e^{L(t-s)} [f(s, (-L)^{-\alpha}x(s)) - f(s, u_0)]\, ds \right\| \\
&\quad + \left\| \int_0^t (-L)^{\alpha} e^{L(t-s)} f(s, u_0)\, ds \right\| \\
&\le \frac{\delta}{2} + \int_0^t c_{\alpha}(t-s)^{-\alpha} L\delta\, ds + \int_0^t c_{\alpha}(t-s)^{-\alpha} B\, ds \\
&= \frac{\delta}{2} + c_{\alpha}(L\delta + B)\frac{t^{1-\alpha}}{1-\alpha} \le \delta.
\end{aligned}$$

This means: F maps S onto itself. Furthermore, we get for $x_1, x_2 \in S$:

$$\begin{aligned}
\|F(x_1)(t) - F(x_2)(t)\| &\le \int_0^t \left\| (-L)^{\alpha} e^{L(t-s)} [f(s, (-L)^{-\alpha}x_1(s)) - f(s, (-L)^{-\alpha}x_2(s))] \right\| ds \\
&\le \int_0^t c_{\alpha}(t-s)^{-\alpha} L \|x_1(s) - x_2(s)\|\, ds \\
&\le c_{\alpha} L \frac{t^{1-\alpha}}{1-\alpha} |x_1 - x_2|_{\chi} \\
&\le \frac{1}{2}\|x_1 - x_2\|_{\chi}.
\end{aligned}$$

just by using the assumption for f and the definition of $\|u\|_{\alpha}$. We have shown now: $F : S \to S$ is a contraction; thus Banach's fixed point theorem yields existence (and uniqueness) of a fixed point $x \in S$ of F.
We take this fixed point x (which satisfies $F(x)(t) = x(t)$) and consider $(-L)^{-\alpha}x$:

$$\begin{aligned}
(-L)^{-\alpha}x &= (-L)^{-\alpha}\left[e^{Lt}(-L)^{\alpha}u_0 + \int_0^t (-L)^{\alpha} e^{L(t-s)} f(s, (-L)^{-\alpha}x(s))\, ds \right] \\
&= e^{Lt}u_0 + \int_0^t e^{L(t-s)} f(s, (-L)^{-\alpha}x(s))\, ds,
\end{aligned}$$

i.e. $(-L)^{-\alpha}x$ is by definition a mild solution of (4.7).
Still to show: it is also a classical solution. Du to $x \in \chi$, the map $t \mapsto f(t, (-L)^{-\alpha}x(t))$ is continuous in $[0, t_0]$. To show: This map is also locally Hölder continuous in $(0, t_0]$.
Let $N = \|f(\cdot, (-L)^{-\alpha}x(\cdot))\|_{\chi}$. For $0 < \beta < 1 - \alpha$ and $0 < h < 1$ the application of Lemma 4 (both inequalities) yields:

$$\begin{aligned}
\|(e^{Lh} - I)(-L)^{\alpha}e^{Lt}\| &\le h^{\beta}\|(-L)^{\beta}(-L)^{\alpha}e^{Lt}\| \\
&= h^{\beta}\|(-L)^{\alpha+\beta}e^{Lt}\| \\
&\le h^{\beta} c_{\alpha+\beta} t^{-(\alpha+\beta)}. \qquad (4.10)
\end{aligned}$$

For $0 < t < t+h \le t_0$ we get

$$\begin{aligned}
\|x(t+h) - x(t)\| &= \|F(x)(t+h) - F(x)(t)\| \\
&\le \|e^{L(t+h)}(-L)^\alpha u_0 - e^{Lt}(-L)^\alpha u_0\| \\
&\quad + \| \int_0^{t+h} (-L)^\alpha e^{L(t+h-s)} f(s,(-L)^{-\alpha}x(s))\,ds \\
&\quad - \int_0^t (-L)^\alpha e^{L(t-s)} f(s,(-L)^{-\alpha}x(s))\,ds\| \\
&\le \|e^{L(t+h)}(-L)^\alpha u_0 - e^{Lt}(-L)^\alpha u_0\| \\
&\quad + \int_0^t \|(-L)^\alpha (e^{Lh} - I) e^{L(t-s)} f(s,(-L)^{-\alpha}x(s))\|\,ds \\
&\quad + \int_t^{t+h} \|(-L)^\alpha e^{L(t+h-s)} f(s,(-L)^{-\alpha}x(s))\|\,ds \\
&=: I_1 + I_2 + I_3.
\end{aligned}$$

Using (4.10) allows us to find estimates for the three terms I_1, I_2, I_3:

$$\begin{aligned}
I_1 &\le c_{\alpha+\beta} h^\beta t^{-(\alpha+\beta)} \|u_0\| \le c_1(t) h^\beta \\
I_2 &\le c_{\alpha+\beta} h^\beta N \int_0^t (t-s)^{-\alpha+\beta)}\,ds \le c_2 h^\beta \\
I_3 &\le c_\alpha N \int_t^{t+h} (t+h-s)^{-\alpha}\,ds = c_\alpha N \frac{h^{1-\alpha}}{1-\alpha} < c_3 h^\beta
\end{aligned}$$

due to $\beta < 1-\alpha$ and $h < 1$.
So, the map $t \mapsto x(t)$ is locally Hölder continuous in $(0, t_0]$. Furthermore we get (due to assumption (NONLIN)):

$$\begin{aligned}
\|f(s,(-L)^{-\alpha}x(s)) - f(t,(-L)^{-\alpha}x(t)\| &\le L(|s-t|^\vartheta + \|x(s) - x(t)\|) \\
&\le L(|s-t|^\vartheta + c|s-t|^\beta),
\end{aligned}$$

which means that also the map $t \mapsto f(t,(-L)^{-\alpha}x(t))$ is locally Hölder continuous in $(0, t_0]$.
From Prop. 4 we know that the linear problem

$$\begin{aligned}
\frac{du}{dt}(t) &= Lu(t) + f(t,(-L)^{-\alpha}x(t)), \qquad \text{for } t > 0 \\
u(0) &= u_0
\end{aligned} \tag{4.11}$$

has a unique classical solution u, which is given by

$$u(t) = e^{Lt}u_0 + \int_0^t e^{L(t-s)} f(s,(-L)^{-\alpha}x(s))\,ds.$$

Now we can apply $(-L)^\alpha$ on this equation and find that

$$(-L)^\alpha u(t) = F(x)(t) = x(t) \quad \Leftrightarrow \quad u(t) = (-L)^{-\alpha}x(t),$$

hence u is a classical solution of (4.7).
Uniqueness of x and uniqueness of the solution of (4.11) provide uniqueness of the desired classical solution.

□

4.4 Existence and uniqueness for reaction-diffusion problems

In this section, we consider a result concerning existence and uniqueness for the problem (4.2-4.4). We do not go into deep details, trying to avoid too much knowledge about Sobolev spaces / embedding / PDE theory, but the basic ideas.

The Sobolev spaces (on the domain $\Omega \subset \mathbb{R}^n$) are defined as follows:

Definition 6 *For $1 \leq p < \infty$ and $k \in \mathbb{N}$*

$$W^{k,p}(\Omega) = \{u \in L^p(\Omega) | \partial^\alpha u \in L^p(\Omega) \quad \forall\, |\alpha| \leq k\}.$$

is called Sobolev space.

The corresponding norm in $W^{k,p}(\Omega)$ is denoted by $\|\cdot\|_{k,p} = \left(\sum_{|\alpha|\leq k} \|\partial^\alpha u\|_{L^p}^p\right)^{\frac{1}{p}}$, then $W^{k,p}(\Omega)$ is a Banach space.

We need to know what an "embedding" means roughly:

Definition 7 *Let $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ be Banach spaces.*

1. *If a linear injective map $j : X \to Y$ exists, then X is called "embedded in Y".*
2. *If this map is also continuous, i.e. for a $c > 0$ it is*

$$\|j(x)\|_Y \leq c\|x\|_X \qquad \forall x \in X,$$

then X is called embedded continuously in Y; this is denoted by $X \hookrightarrow Y$.

Remark: If X is embedded continuously in Y, then each element of X can be identified uniquely with an element of Y (interpret X as subspace of Y and write $X \subseteq Y$).

The first propositions yields a regularity result for solutions of elliptic boundary problems (we consider the elliptic operator $L = \Delta$):

Proposition 5 *There exists a constant $c > 0$ with*

$$\|u\|_{2,2} \leq c\|Lu\|_{0,2}.$$

So, the operator L satisfies the conditions of the section concerning the abstract linear problems for $\mathcal{H} = L^2(\Omega)$; and we can define $(-L)^\alpha$ and $\mathcal{H}_a$ as in the section concerning the abstract semilinear problems.
One can show the following embedding results:

Proposition 6 *Let $0 < \alpha \leq 1$.*

a) For $k - \frac{n}{p} < 2\alpha - \frac{n}{2}$ and $p \geq 2$ it is $\mathcal{H}_\alpha \hookrightarrow W^{k,p}(\Omega)$

b) For $0 \leq \nu < 2\alpha - \frac{n}{2}$ it is $\mathcal{H}_\alpha \hookrightarrow C^\nu(\bar{\Omega})$.

Now we can formulate a proposition concerning existence and uniqueness (case $n \leq 3$).

Proposition 7 *Let $\Omega \subset \mathbb{R}^n$ a bounded domain with smooth boundary, where $n \leq 3$. Assume that for the function $f : [0,T] \times \Omega \times \mathbb{R}^m \times \mathbb{R}^{3m} \to \mathbb{R}^m$ a continuous function $\rho : [0,T] \times [0,\infty) \to [0,\infty)$ exists, which is monotonously increasing in the second argument, a constant $1 \leq \gamma < 3$ and a $\vartheta \in (0,1]$ exist, such that*

$$\begin{aligned}
|f(t,x,u,p)| &\leq \rho(t,|u|)(1+|p|^\gamma), && (4.12)\\
|f(s,x,u,p) - f(t,x,u,p)| &\leq \rho(0,|u|)(1+|p|^\gamma)|s-t|^\vartheta && (4.13)\\
|f(t,x,u,p) - f(t,x,u,q)| &\leq \rho(t,|u|)(1+|p|^{\gamma-1}+|q|^{\gamma-1})|p-q| && (4.14)\\
|f(t,x,u,p) - f(t,x,v,p)| &\leq \rho(t,|u|+|v|)(1+|p|^\gamma)|u-v|. && (4.15)
\end{aligned}$$

Furthermore, let the map $x \mapsto f(t,x,u,p)$ be measurable.
Then, there exists for each $u_0 \in H^2(\Omega) \cap H_0^1(\Omega)$ a $t_0 > 0$, such that problem (4.2)-(4.4) has a unique classical solution in $[0,t_0)$.

Rough idea of the proof: If α is chosen in such a way that $\max\{\frac{3}{4}, \frac{5\gamma-3}{4\gamma}\} < \alpha < 1$, then proposition 6 yields

$$\mathcal{H}\alpha \subset W^{1,2\gamma}(\Omega) \cap L^\infty(\Omega)$$

One can show that F with $F(t,u)(x) = f(t,x,u(x),\nabla u(x))$ satisfies assumption (NONLIN), which allows to apply theorem 12. This yields directly the assertion of this proposition.

Remark: For the special cases $n = 1$ and $n = 2$ "better" statements are possible, e.g. concerning conditions for the nonlinearity.

4.5 Global solutions

As an auxiliary result, we use a generalisation of the lemma of Gronwall (probably known in a simpler version for ODEs):

Lemma 5 (Lemma of Gronwall) *Let $a, b \geq 0$, $0 \leq \alpha, \beta < 1$ and $0 < T < \infty$. Then, there exists a constant $M = M(b, \alpha, \beta, T)$, such that for each integrable function $u : [0, T] \to \mathbb{R}$, which satisfies*

$$0 \leq u(t) \leq at^{-\alpha} + b \int_0^t (t-s)^{-\beta} u(s)\, ds \qquad \text{for } 0 \leq t \leq T,$$

it is

$$u(t) \leq aMt^{-\alpha} \qquad \text{for } 0 \leq t \leq T.$$

Now we deal with the global existence of a solution, i.e. for all $t > 0$.

Proposition 8 *Let the assumption (NONLIN) be satisfied with $T = \infty$ and $U = \mathcal{H}_\alpha$. Let u be a solution of (4.7) (the abstract semilinear model, $\frac{du}{dt}(t) = Lu(t) + f(t, u(t))$ ...) such that*

$$\|f(t, u(t))\| \leq K(t)(1 + \|u(t)\|_\alpha)$$

for all t, for which the solution exists; $K : [0, \infty) \to \mathbb{R}$ is a continuous function. Then the solution of (4.7) exists for all $t > 0$.

Rough idea for the proof: By using the representation

$$u(\tau) = e^{L\tau} u_0 + \int_0^\tau e^{L(\tau - s)} f(s, u(s))\, ds$$

one gets an estimate of the form

$$\|u(\tau)\|_\alpha \leq M_1(t) + M_2(t) \int_0^\tau (\tau - s)^{-\alpha} \|u(s)\|_\alpha\, ds.$$

This can be rewritten in such a way that the assumptions of the Gronwall Lemma are satisfied, and this yields

$$\|u(t)\|_\alpha \leq M(t)$$

for all t, for which the solution u exists.
The assumption of a bounded interval of existence leads to contradiction (via mild solution which is also a classical solution).

(□)

Hence, is the nonlinearity grows maximally linear (along the solution), one gets global existence.

Chapter 5

Stationary solutions / Stability

Reference: [1]

5.1 Basics

We have seen statements concerning the existence of solutions, also the global existence, i.e. which exist for all time. So, a natural question is about the asymptotic behaviour of solutions for $t \to \infty$.

We start with a simple (scalar) 1D reaction diffusion equation with homogeneous Neumann boundary conditions:

$$\begin{aligned} u_t &= u_{xx} + f(u) \qquad \text{in } \Omega \times (0,\infty) && (5.1)\\ \frac{\partial u}{\partial n} &= 0 \qquad \text{on } \partial\Omega \times (0,\infty), && (5.2) \end{aligned}$$

where Ω is a bounded interval; additionally, initial conditions have to be prescribed; f is assumed to be sufficiently smooth.

A stationary solution means (obviously) that it doesn't change in time, thus it can be written as $u(x,t) = v(x)$. Inserting this approach into (5.1),(5.2) yields

$$v'' + f(v) = 0 \quad \text{in } \Omega, \qquad v' = 0 \quad \text{on } \partial\Omega,$$

i.e. an ODE problem with boundary conditions.
This second order ODE can be easily transformed into a 2D system of first order ODEs by introducing $w = v'$:

$$\begin{aligned} v' &= w \\ w' &= -f(v). \end{aligned}$$

The so-called energy integral can be introduced (quite similar to a Lyapunov function), let

$$E(v,w) = \frac{w^2}{2} + F(v) + const..$$

It satisfies:

$$\begin{aligned} E' = \frac{d}{dx}E(v,w) &= \frac{\partial E}{\partial v}v' + \frac{\partial E}{\partial w}\dot{w} \\ &= f(v)\cdot w + w\cdot(-f(v)) = 0. \end{aligned}$$

Indeed, E stays constant along solution curves (v,w). How does the phase plane diagram look like? This depends on the chosen f!
Special case: We consider f satisfying

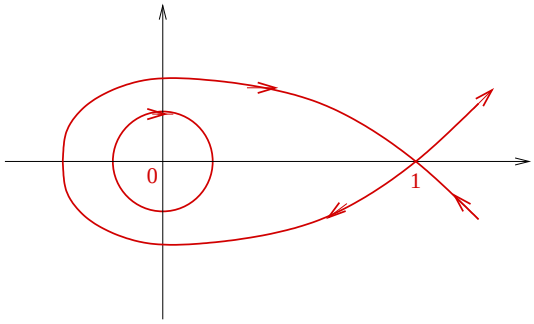
$$f(0) = 0 = f(1) \qquad \text{with } f > 0 \text{ in } (0,1), \tag{5.3}$$

$$f'(0) > 0, \qquad f'(1) < 1. \tag{5.4}$$

An example for such a f is the logistic growth as reaction term (the whole PDE (5.1) is called then "Fisher equation"; here we have a "generalised Fisher equation"). The stationary points are easy to determine:

$$(v, w) = (0, 0) \text{ and } (v, w) = (1, 0).$$

For checking the stability / type of stationary point, the linearisation is partially useful: For $(1, 0)$ we get a saddle point; but for $(0, 0)$ the theorem of Hartman-Grobman is not applicable. But we can use the level sets of $E(v, w)$: Obviously, the system is symmetric with respect to the x-axis, so near $(0, 0)$, there will be closed orbits. The phase plane looks as follows:



For solutions of the Neumann problem it is necessary that they start and end at $v' = 0$, i.e. at $w = 0$, which correspond to points on the v-axis. On can formulate the following statement:

Proposition 9 *For the stationary problem of the generalised Fisher equation (5.1), (5.2), with (5.3), (5.4), zero-flux boundary conditions, Ω a bounded interval, two solutions exist with $0 \le u \le 1$: $u = 0$ and $u = 1$. For continuous intial conditions*

$$u(x, 0) = u_0(x), \qquad 0 \le u_0 \le 1,$$

the solution satisfies

$$\lim_{t \to \infty} u(x, t) = 1,$$

uniformly in $x \in \bar{\Omega}$; except for $u = 0$, if $u_0 = 0$ (everywhere).

Idea of the proof: Obviously, the only stationary points are $(0, 0)$ and $(1, 0)$. If $u_0 = 0$, then also $u = 0$ (due to the stationarity). It remains to show that $u_0 \neq 0$ leads to $u \to 1$ for $t \to \infty$. This can be done by using the comparison principle in a slightly modified version for Neumann conditions.

$(\square)$

It is even possible to show the same statement for a reaction term f which satisfies

$$f(0) = 0 = f(1), \qquad f > 0 \text{ in } (0, 1), \qquad f'(0) = 0 \text{ and } f'(1) < 0.$$

We already met the Allee effect (this type of approach is also called "generalised Nagumo equation" or "bistable equation"); in this case f satisfies the conditions

$$f(0) = f(a) = f(1) = 0, \qquad f < 0 \text{ in } (0, a), \qquad f > 0 \text{ in } (a, 1).$$

How does the phase plane look like in this case? And what are the consequences for solutions of the Neumann-problem? For simplicity, we choose concretely $f(u) = u(1 - u)(u - a)$ where $0 < a < \frac{1}{2}$. $\rightsquigarrow$ see exercises!

5.2 Example: The spruce budworm model

(see [1] for some more details;
some background information can be found at http://www.unbf.ca/forestry/centers/cwru/patch.htm)

The spruce-budworm is a caterpillar of a moth which defoliates spruce stands in Canada.
Situation:

- epidemic spread-out
- large damages in the forest during heavy epidemics
- in the situation of large damages, the population falls onto a low, but endemic level.
- outbreaks occur in intervals of 30-40 years

But if the woodland is small enough, it is not possible to establish a stable surviving population. So the question arises about the maximal size of a woodland which does not allow a stable settling of the budworms.

The original model which was introduced by Ludwig et al. in 1978 reads as follows (in its nondimensionalised form):

$$u_t = u(1-u) - \frac{1}{R}\frac{u^2}{\varepsilon^2+u^2} + u_{xx}.$$

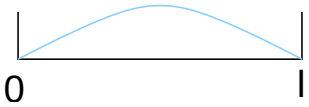
R denotes a parameter for the amount of foliage available (assumed constant for the model time-scale). The term $-\frac{u^2}{R(\varepsilon^2+u^2)}$ describes effects of predation and parasitism on the budworm population; ε is a constant small parameter. In the following, we use Fisher's equation:

$$u_t = Du_{xx} + \mu u(1-u), \tag{5.5}$$

where $u(t,x)$ describes the population density; spread-out by diffusion, logistic growth (the term which describes predation / parasitism on the budworm population is neglected here).

Consider a woodland in the interval $[0,l]$. For a PDE on a bounded interval, it is necessary to introduce boundary conditions. For the application considered here, it is reasonable to use homogeneous Dirichlet boundary conditions,

$$u(0,t) = 0, \quad u(l,t) = 0,$$



since outside of the woodland, the budworms cannot live; thus, there is $u = 0$.

The question about the minimal interval size to support a population has been shown to be equivalent to the question, when the trivial solution $u(x,t) = 0$ is unstable (in case of a stable $u(x,t) \equiv 0$, each solution near 0 would tend to 0 and lead to extinction), see e.g. [1].
For Fisher's equation, it is again equivalent to search for the critical domain length l^* such that a non-trivial steady state exists for $l > l^*$. We look for stationary solutions (with $u_t = 0$), thus

$$u_{xx} = -\frac{\mu}{D}u(1-u)$$

with $u(0) = 0$, $u(l) = 0$.
Introducing a new variable $v := u_x$ leads to the following ODE system:

$$\begin{aligned} u_x &= u' = v \\ v_x &= v' = -\frac{\mu}{D}u(1-u) \end{aligned}$$

(Remark here, there are derivatives with respect to x, not to time t as often usual).
The usual analysis of such an ODE-system yields:

- Stationary points $P_1 = (0,0)$, $P_2 = (1,0)$
- General Jacobian matrix: $Df(u,v) = \begin{pmatrix} 0 & 1 \\ -\frac{\mu}{D} + 2\frac{\mu}{D}u & 0 \end{pmatrix}$
- Eigenvalues of the Jacobian matrix in the stationary points:

$$\begin{aligned} Df(0,0): &\quad \begin{pmatrix} 0 & 1 \\ -\frac{\mu}{D} & 0 \end{pmatrix}, \quad \lambda_{1,2} = \pm i\sqrt{\frac{\mu}{D}} \qquad \text{centre} \\ Df(1,0): &\quad \begin{pmatrix} 0 & 1 \\ \frac{\mu}{D} & 0 \end{pmatrix}, \quad \lambda_{1,2} = \pm\sqrt{\frac{\mu}{D}} \qquad \text{saddle} \end{aligned}$$

We have to check, if also the nonlinear system has a centre in $(0,0)$ (Hartman-Grobman theorem cannot be applied).
Here, it is very useful to introduce a Hamiltonian function to check for that.
A Hamiltonian function has to satisfy

$$\frac{\partial H}{\partial v} = u' \quad \text{and} \quad \frac{\partial H}{\partial u} = -v', \tag{5.6}$$

so for solution $(u(x), v(x))$ of the original system, we get

$$\frac{d}{dx} H(u(x), v(x)) = \frac{\partial H}{\partial u} u' + \frac{\partial H}{\partial v} v' = -v'u' + u'v' = 0. \tag{5.7}$$

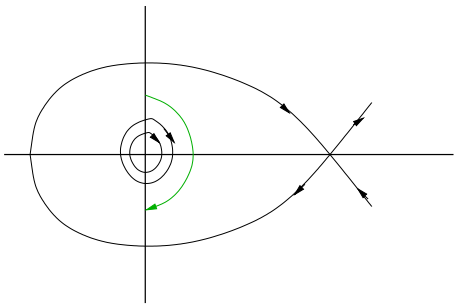
Condition (5.6) and property (5.7) are the defining properties for H to be a Hamiltonian function (of the corresponding ODE system). Obviously, (5.7) means, that H does not change along solution curves $(u(x), v(x))$, so the solution curves lie on level lines of H.
In our example, we can define a Hamiltonian function as follows:

$$H(u,v) = \frac{1}{2}v^2 + \frac{\mu}{D}\frac{u^2}{2} - \frac{\mu}{D}\frac{u^3}{3}$$

(it is easy to check, that (5.6) and (5.7) are satisfied). Certain properties of a Hamiltonian function yield, that for each bounded solution, there are only three possibilities: it is

- an equilibrium point, or
- a connection of equilibrium points, or
- a closed orbit

Now, we have to recall the boundary conditions; we look for a solution that starts in 0 ($u(0) = 0$) and connects to $u(l) = 0$, while it stays nonnegative in between. Such a solution looks as follows:



There is a unique u-axis intersection point u^* for each solution. If we let tend $u^* \to 1$, then the solution would approach the saddle point, but very close to the saddle point, the motion becomes "more slowly" and "more slowly", i.e. $l \to \infty$ for $u^* \to 1$.
Surprisingly, it is not true that $l \to 0$ for $u^* \to 0$. For $u^* \to 0$, we are in the range close to $(0,0)$, where mainly the linearisation influences the behaviour of the solutions. The linearisation yielded a centre at $(0,0)$ with the eigenvalues $\lambda_{1,2} = \pm i\sqrt{\frac{\mu}{D}}$, so the solution near $(0,0)$ is approximately given by

$$\begin{pmatrix} u(x) \\ v(x) \end{pmatrix} = \begin{pmatrix} c_1 \sin(\sqrt{\frac{\mu}{D}}x) \\ c_2 \cos(\sqrt{\frac{\mu}{D}}x) \end{pmatrix}.$$

Looking for a Dirichlet solution, we need a half circle starting at $x_0 = 0$, where $\pi = \sqrt{\frac{\mu}{D}}l$, thus $l = \pi\sqrt{\frac{D}{\mu}}$.
So, the critical patch size in the limit $u^* \to 0$ reads $l_c = \pi\sqrt{\frac{D}{\mu}}$.

A bit more precise: We look for a steady state solution with $u(0) = 0 = u(l)$. By symmetry, we get $u(\frac{l}{2}) =: u^*$, $v(\frac{l}{2}) = 0$; it is $u^* < 1$ (no solution curve can pass through the saddle point $(1,0)$. It is also $v(0) = u'(0) > 0$ and $v(l) = u'(l) < 0$. Take the equation $u'' + \frac{\mu}{D}u(1-u) = 0$ in $0 < x < l$, multiply it by u' and obtain

$$u'u'' + \frac{\mu}{D}u(1-u)u' = 0.$$

Integrating this equation yields

$$\frac{u'^2}{2} + \underbrace{\frac{\mu}{D}\frac{u^2}{2} - \frac{\mu}{D}\frac{u^3}{3}}_{=:F(u)} = \underbrace{A}_{=:F(u^*)} \ (= const.)$$

(the integration constant can be chosen arbitrarily, hence also as $F(u^*)$).
This can be solved for u':

$$u' = \begin{cases} \sqrt{2(F(u^*) - F(u))} & \text{for } 0 \le x \le \frac{l}{2} \\ -\sqrt{2(F(u^*) - F(u))} & \text{for } \frac{l}{2} \le x \le l, \end{cases}$$

then the sign of u' fits to the requirement.
Integrating this from x to $\frac{l}{2}$ yields (for $0 < x < \frac{l}{2}$):

$$\begin{aligned} \frac{l}{2} - x = \int_x^{\frac{l}{2}} 1\,dy &= \int_x^{\frac{l}{2}} \frac{u'}{\sqrt{2(F(u^*) - F(u))}}\,dy \\ &= \int_{u(x)}^{u(\frac{l}{2})} \frac{1}{\sqrt{2(F(u^*) - F(z))}}\,dz \\ &= \int_{u(x)}^{u^*} \frac{1}{\sqrt{2(F(u^*) - F(z))}}\,dz. \end{aligned}$$

For $\frac{l}{2} < x < l$ we get similarly by integrating

$$\begin{aligned} \int_x^{\frac{l}{2}} -\frac{u'}{\sqrt{2(F(u^*) - F(u))}}\,dy &= \int_x^{\frac{l}{2}} 1\,dy \\ \Leftrightarrow \qquad \int_{u(x)}^{u^*} \frac{1}{\sqrt{2(F(u^*) - F(z))}}\,dz &= x - \frac{l}{2}, \end{aligned}$$

which corresponds to (in general)

$$\int_{u(x)}^{u^*} \frac{1}{\sqrt{2(F(u^*) - F(z))}}\,dz = \left| x - \frac{l}{2} \right|.$$

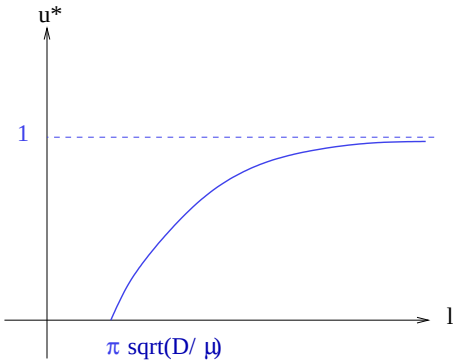
If μ is known, this is an implicit equation for u.
The boundary conditions claim $u(0) = u(l) = 0$, hence for $x = 0$ and/or $x = l$:

$$\int_0^{u^*} \frac{1}{\sqrt{2(F(u^*) - F(z))}}\,dz = \frac{l}{2} \qquad \Leftrightarrow \qquad l = \sqrt{2}\int_0^{u^*} \frac{1}{\sqrt{F(u^*) - F(z)}}\,dz.$$

Due to monotonicity etc., the length l of the domain uniquely determines u^*. It can be interpreted as "given a non-trivial solution with max. value u^*, how long is the corresponding length l of the domain?"
Minimally, we can have $u^* \to 0$. So we determine

$$\begin{aligned} l_c &= \lim_{u^* \to 0} \sqrt{2}\int_0^{u^*} \frac{1}{\sqrt{F(u^*) - F(z)}}\,dz \\ &= \lim_{u^* \to 0} \sqrt{2}\int_0^{u^*} \frac{1}{\sqrt{-\frac{\mu}{D}\frac{z^2}{2} + \frac{\mu}{D}\frac{z^3}{3} + \frac{\mu}{D}\frac{u^{*2}}{2} - \frac{\mu}{D}\frac{u^{*3}}{3}}}\,dz \\ &= \lim_{u^* \to 0} \frac{2}{\sqrt{\frac{\mu}{D}}}\int_0^{u^*} \frac{1}{\sqrt{-z^2 + \frac{2}{3}z^3 + u^{*2} - \frac{2}{3}u^{*3}}}\,dz \\ &= \lim_{u^* \to 0} 2\sqrt{\frac{D}{\mu}}\int_0^{u^*} \frac{dz}{\sqrt{u^{*2} - z^2}} \\ &= \lim_{u^* \to 0} 2\sqrt{\frac{D}{\mu}}\left[\arcsin\frac{z}{u^*}\right]_0^{u^*} \\ &= \sqrt{\frac{D}{\mu}}\pi. \end{aligned}$$

The graph of u^*, dependent on l looks as follows:



□

Until now, we know conditions for the existence of a non-trivial stationary solution (which is denoted by $\tilde{u}(x)$ in the following), but not if a time-dependent solution will tend to this stationary solution. The following theorem gives information about that:

Theorem 13 *We consider $u_t = u_{xx} + u(1-u)$ with homogeneous Dirichlet boundary conditions $u(0,t) = 0 = u(l,t)$ and positive initial conditions*

$$u(x,0) = u_0(x) > 0 \qquad \text{in } (0,l)$$

Then it holds

(i) If $0 < l < \pi$, then $u(x,t) \to 0$ for $t \to \infty$

(ii) If $l > \pi$, then $u(x,t) \to u(x)$ (the non-trivial stationary solution) for $t \to \infty$.

(Idea of the) Proof :

(i) The comparison theorem is useful: $\underline{u} = 0$ can be chosen as subsolution. In the next step, we try to find a supersolution $\bar{u}$ which tends to 0 for $t \to \infty$. Let $\bar{u}$ be the solution of

$$\bar{u}_t = \bar{u} + \bar{u}_{xx} \qquad \text{in } 0 < x < l, \;\; t > 0$$

with the boundary conditions

$$\bar{u}(0,t) = 0 \quad \text{and} \quad \bar{u}(l,t) = 0$$

and the initial condition

$$\bar{u}(x,0) = u_0(x)$$

Let $Nu = u_t - u_{xx} - u(1-u)$ (for a general u), then it holds that

$$N\bar{u} = \bar{u}_t - \bar{u}_{xx} - \bar{u}(1-\bar{u}) = \bar{u}^2 \geq 0 = Nu.$$

On the boundaries and the initial interval, we have $\bar{u} = u$, so the comparison theorem can be applied again and yields

$$u(x,t) \leq \bar{u}(x,t)$$

everywhere. Using what we have seen already in the example for the separation of variables (in a slight modification), it is $\bar{u}(x,t) \to 0$ for $t \to \infty$ in case of $l < \pi$, hence also

$$u(x,t) \to 0 \qquad \text{for } t \to \infty.$$

(ii) In this case, we are interested in sub- and supersolutions which both bend to the stationary solution $\tilde{u}(x)$. Again we use the nonlinear operator N as $Nu = u_t - u(1-u) - u_{xx}$. We define

$$M_0 = \sup_{0 \leq x \leq l} u_0(x), \qquad M = \max\{1, M_0\}.$$

Let $\bar{u}$ be the solution of

$$\begin{aligned} N\bar{u} &= 0 \qquad \text{for } 0 < x < l, \;\; t > 0, \\ \bar{u}(x,0) &= M \qquad \text{for } 0 < x < l, \\ \bar{u}(0,t) = 0 \quad &\text{and} \quad \bar{u}(l,t) = 0 \qquad t > 0. \end{aligned}$$

This solution $\bar{u}$ satisfies $N\bar{u} = 0 \geq 0 = Nu$, $\bar{u}(0,t) = 0 \geq 0 = u(0,t)$, $\bar{u}(l,t) = 0 \geq 0 = u(l,t)$ and $\bar{u}(x,0) = M \geq M_0 \geq u(x,0)$; hence $\bar{u}$ is indeed a supersolution of the problem for u and we get that $\bar{u}(x,t) \geq u(x,t)$ for $0 \leq x \leq l$ and $t \geq 0$ by the comparison theorem. In the next step we need to show that $\bar{u}$ is monotone decreasing (and hence tends to a limit), i.e. $\bar{u}(x,t) \geq \bar{u}(x,t+h)$. Define $U_h(x,t) = \bar{u}(x,t)$ for any fixed h. U_h satisfies:

$$\begin{aligned} NU_h &= 0 \qquad \text{for } 0 < x < l, \ t > 0 \\ U_h(x,0) &= \bar{u}(x,h) \qquad \text{for } 0 < x < l \\ U_h(0,t) = 0 \quad &\text{and} \quad U_h(l,t) = 0 \qquad \text{for } t > 0. \end{aligned}$$

Hence, U_h is a subsolution of the problem for $\bar{u}$ in case of $U_h(x,0) \leq \bar{u}(x,0)$. Due to $\bar{u}(x,t) \leq M$ for all t, it is also

$$U_h(x,0) = \bar{u}(x,h) \leq M = \bar{u}(x,0),$$

and it follows that

$$\bar{u}(x,t+h) = U_h(x,t) \leq \bar{u}(x,t) \qquad \text{for all} x,t,$$

i.e. $\bar{u}$ is monotone decreasing. As it is bounded below by zero, $\lim_{t\to\infty} \bar{u}(x,t) = w(x)$ exists and it is $0 \leq w(x) \leq M$. With some more analytical tools one can show (see Aronson and Weinberger, 1975, 1978) that indeed $w(x)$ is a non-negative solution of $u_t = u(1-u) + u_{xx}$ satisfying the boundary conditions $u(0,t) = u(l,t) = 0$.
Next, it is necessary to show that w is non-zero: Remember that there is a unique positive solution $u(x)$; so we can use the comparison theorem (it is $Nu = 0$ with zero boundary conditions and initial conditions $u(x) \leq 1 \leq M = \bar{u}(x,0)$), which yields $\bar{u}(x,t) = u(x)$, thus also $w(x) \geq u(x)$. But $u(x)$ is the unique positive solution of the given problem, so it follows that

$$w(x) = u(x), \quad \rightsquigarrow \quad \lim_{t\to\infty} \bar{u}(x,t) = u(x).$$

In a similar, but slightly more complicated way, one can construct a subsolution $\underline{u}(x,t)$ which bounds $u(x,t)$ from below. For this subsolution $\underline{u}(x,t)$ it can be shown that

$$\lim_{t\to\infty} \underline{u}(x,t) = u(x).$$

Altogether, this yields $\underline{u} \leq u \leq \tilde{u}$ and

$$\lim_{t\to\infty} u(x,t) = u(x).$$

This means that for $l > \pi$, the stationary solution $u(x,t) = u(x)$ of the logistic equation in $(0,l)$ with zero boundary conditions and positive initial conditions is globally attracting.

□

For the original spruce-budworm model, similar calculations can be done (just more complex) and yield finally

Theorem 14 *For the spruce-budworm equation,*

$$u_t = u(1-u) - \frac{1}{R}\frac{u^2}{\varepsilon^2 + u^2} + u_{xx} \qquad \textit{for } x \in (0,l),$$

with the boundary conditions

$$u(0,t) = 0 = u(l,t),$$

no stationary solutions exists if $l < \pi$. In case of $l > \pi$, there are stationary solutions of the following form:

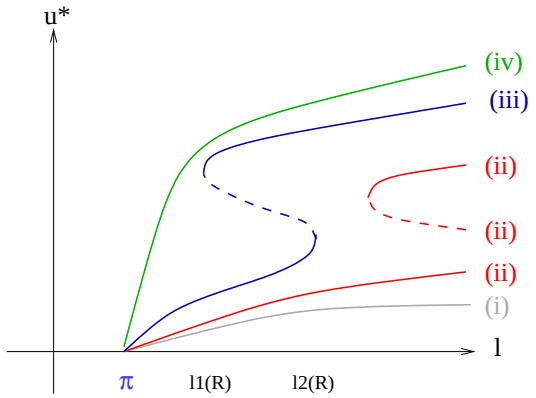
(i) For small R ($R < R_1$), there exists one non-trivial solution, which is at endemic level and stable.

(ii) For larger R ($R_1 < R < R_2$), the stable solution at the endemic level still exists for all $l > \pi$, but for $l > l_1(R)$ a second stable solution appears at the so-called epidemic level; between these two stable solutions, there is an unstable solution.

(iii) For larger R ($R_2 < R < R_3$), the solution at the endemic level disappears for $l > l_2(R)$. (It depends on the initial conditions to which stable solution the solution tends to)

(iv) For the largest R ($R > R_3$), the solution tends to the stable epidemic level if l increases through π.

The corresponding bifurcations diagram looks as follows:



Application of the mathematical theorem:
The basic idea is always to prevent an outbreak of an epidemic

- In case of $R > R_3$ (trees healthy, foliage abundant), the only chance for prevention is to have strips of forest of width $< \pi$ (in original variables $\pi\sqrt{D/r}$ with r per capita growth rate of budworm for small population density)
- In case of $R_1 < R < R_3$, the critical length below which an epidemic cannot happen is larger: $l_1(R)$ (in original variables $l_1(R)\sqrt{D/r}$).

Until now, we considered 1D spatial situations. Of course, also higher dimensions are of interest, e.g. consider

$$u_t = \Delta u + kf(u) \qquad \text{in } \Omega \times (0, \infty)$$

with $\Omega \subset \mathbb{R}^n$ bounded domain, k a parameter; boundary conditions

$$u = 0 \qquad \text{on } \partial\Omega \times (0, \infty)$$

and initial conditions.
In the 1D case, we kept k constant and varied the size of the domain; of course, one can also keep Ω "fixed" and vary k. k can be interpreted as a measure of the domain size.
Let L be the Laplace operator on Ω with homogeneous Dirichlet boundary conditions. Classical results of the spectral theory of L may help us.

Definition 8 *The spectrum of L, denoted by $\sigma(L)$, is the set*

$$\{\lambda \in \mathbb{C} | L - \lambda I \text{ is not invertible } \}$$

Proposition 10 *For L as introduced above it holds:*

(a) $\sigma(L)$ is discrete and consists only of real negative eigenvalues

(b) L has a unique positive eigenfunction, which corresponds to the largest eigenvalue (denoted by ϕ and $\lambda_0 = \lambda_0(k)$, called principal eigenfunction / principal eigenvalue)

(c) If $k_1 > k_2$, then $\lambda_0(k_1) > \lambda_0(k_2)$ (i.e. the principal eigenvalue depends monotonically on the domain)

(d) λ_0 is a continuous function of k (i.e. the principal eigenvalue depends continuously on the domain)

Proof: see e.g. [14]

As a quite simple example (for a reaction-diffusion equation) we consider the linear problem

$$\begin{aligned} u_t &= \Delta u + ku \qquad \text{in } \Omega \times (0, \infty) \\ u &= 0 \qquad \text{on } \partial\Omega \times (0, \infty) \end{aligned}$$

Let λ_i be the eigenvalues of L, then the eigenvalues of the linear problem are given by $\mu_i = k + \lambda_i$. Then the largest eigenvalue is $k + \lambda_0(k)$.
Let's have a short excurs to linear problems, written as

$$v_t = Av,$$

where A is a linear differential operator defined on a suitable function space which satisfies the prescribed boundary conditions. As in the preceding chapter, the definition domain of A, $D(A)$ can be extended to a dense subset of an Banach space X (e.g. $L_2(\Omega)$), which allows us to use the X-Norm. An steady state u_0 is asymptotically stable, if $\|v\|_X \to 0$ for $t \to \infty$. If the spectrum of A is contained completely in the left half space of the complex plane (i.e. $Re(\lambda) \leq \beta$ for a $\beta < 0$ for all $\lambda \in \sigma(A)$). One can show that in this case $\|v\|_X$ decays like $e^{\beta t}$. The idea behind is easy to see: For simple initial-boundary-value problems on compact domains, $\sigma(A)$ consists of a sequence of eigenvalues $\{\lambda_m\}$, with corresponding eigenfunctions which satisfy

$$A\phi_m = \lambda\phi_m.$$

If there exists a $m \in \mathbb{N}$ such that $Re(\lambda_m) \geq 0$, then we get for an initial condition of the form

$$v(x,0) = const \cdot \phi_m(x)$$

the solution

$$v(x,t) = const \cdot e^{\lambda_m t}\phi_m(x).$$

But such a $v(x,t)$ does not approach zero for $t \to \infty$, i.e. zero is unstable in this case.
Vice versa: As already known, the function space which contains the solutions v is spanned by the eigenfunctions, any solution can be written in the following way:

$$v(x,t) = \sum_{m=1}^{\infty} a_m(t)\phi_m(x).$$

This leads (via $v_t = Av$) to the condition for the coefficients $a_m(t)$:

$$\frac{da_m}{dt} = \lambda_m a_m$$

Hence $\lambda_m < 0$ is needed for each m to get $v \to 0$ for $t \to \infty$.
(Remark that similar considerations can be done in case of an unbounded Ω, but becomes more complicated due to a more complicated spectrum - not only with discrete eigenvalues, such a continuum is called "essential spectrum", but the latter one depends essentially on the choice of function space for possible initial values for v)

Back to our problem $u_t = \Delta u + ku$; now we know:
If $\lambda_0(k) < -k$ (which corresponds to a sufficiently small domain Ω), then all eigenvalues μ are negative, resulting in a stable steady state 0.
If $\lambda_0(k) > -k$ (which corresponds to a sufficiently large domain Ω), then $\mu_0 = k + \lambda_0(k) > 0$ and the steady state is unstable.

In the next step, we show that the stability of the trivial solution of a corresponding nonlinear problem can be examined by a linear stability analysis (somehow analogous to Hartman-Grobman theorem for ODEs).

Theorem 15 (Principle of Linearised Stability) *Consider*

$$\begin{aligned} u_t &= \Delta u + ku + h(u) \qquad \text{in } \Omega \times (0,\infty) \\ u &= 0 \qquad \text{on } \partial\Omega \times (0,\infty) \\ u(x,0) &= u_0(x), \end{aligned}$$

where $h(0) = 0$, $h'(0) = 0$. Let $\lambda_0 = \lambda_0(k)$ be the principal eigenvalue in $\sigma(L)$.
If $\lambda_0 < -k$, then the trivial steady state is stable.
If $\lambda_0 > -k$, then it is unstable.

Proof: Let $\lambda_0 < -k$. We aim to find a supersolution of the problem which tends to zero for $t \to \infty$. From Prop. 10 it is known: the principal eigenvalue of L depends continuously and monotonically on the domain (k), so it is possible to find a $k' > k$ satisfying $\lambda_0(k) < \lambda_0(k') < -k$. Let $\bar{u}(x,t)$ be the solution of

$$\begin{aligned} \bar{u}_t &= \Delta\bar{u} + k'\bar{u} \qquad \text{in } \Omega \times (0,\infty) \\ \bar{u} &= 0 \qquad \text{on } \partial\Omega \times (0,\infty) \\ \bar{u}(x,0) &= u_0(x) \end{aligned}$$

Considering the eigenvalues of this problem yields that $\bar{u}$ is monotone decreasing and indeed tends to zero for $t \to \infty$. Due to the definitions we find:

$$N\bar{u} = \bar{u}_t - k\bar{u} - h(\bar{u}) - \Delta\bar{u} = (k'-k)\bar{u} - h(\bar{u}).$$

It is $k' > k$, so there exists a $\varepsilon > 0$ such that

$$(k'-k)u - h(u) \geq 0 \qquad \forall u \in (0,\varepsilon)$$

If u_0 satisfies the inequality $u_0(x) \leq \varepsilon$ for all $x \in \Omega$, then we get $\bar{u}(x,t) \leq u_0(x) \leq \varepsilon$ (as $\bar{u}$ is monotone decreasing) and

$$N\bar{u} \geq 0$$

(due to $(k'-k)\bar{u} - h(\bar{u}) \geq 0$)
Hence, $\bar{u}$ is a supersolution of the problem for u which tends to zero; we get that the trivial solution is indeed asymptotically stable.

The instability of the trivial solution in case of $\lambda_0 > -k$ can be shown in a similar way (left out here).

□

By such an approach, the existence of a non-trivial steady state solution for the logistic equation can be shown:

Theorem 16 *If $\lambda_0 > -k$, then*

$$\begin{aligned} u_t &= \Delta u + ku(1-u) \qquad \textit{in } \Omega \times (0,\infty) \\ u &= 0 \qquad \textit{on } \partial\Omega \times (0,\infty) \end{aligned}$$

possesses at least one non-trivial nonnegative steady state solution.

Idea of the proof: Again we use sup- and supersolutions. Let $\delta > 0$ and let ϕ be the principal eigenfunction of L, i.e. $\Delta\phi = \lambda_0\phi$ with $\lambda_0 + k > 0$ (according to the assumption), $\phi > 0$ in Ω (according to Prop. 10) and $\phi = 0$ on $\partial\Omega$.
Let $\underline{u} = \delta\phi$, then it satisfies

$$\begin{aligned} \underline{u}_t - k\underline{u}(1-\underline{u}) - \Delta\underline{u} &= -\lambda_0\delta\phi - k\delta\phi(1-\delta\phi) \\ &= -(\lambda_0 + k)\delta\phi + \delta^2 k\phi^2 \\ &\leq 0 \end{aligned}$$

for a sufficiently small δ; of course $\underline{u} = 0$ on $\partial\Omega \times (0,\infty)$, so $\underline{u}$ is a subsolution.
For a supersolution we can take $\bar{u} = 1$. Obviously it is

$$N\bar{u} = \bar{u}_t - \Delta\bar{u} - k\bar{u}(1-\bar{u}) = 0 \qquad \text{in } \Omega$$

and $\bar{u} \geq 0$ on $\partial\Omega \times (0,\infty)$. Similar to Theorem 13, the existence of a steady-state solution $v(x)$ with $\underline{u}(x) \leq v(x) \leq \bar{u}(x)$ can be shown.

(□)

Remark: For the budworm equation, a similar statement can be shown.

Chapter 6

Reaction-diffusion systems

6.1 What can be expected from Reaction-diffusion systems?

Reference. [12]

In general, systems of reaction-diffusion equations allow for much more complex behaviour than a scalar reaction-diffusion equation does. Especially interacting reaction terms are of interest and lead to interesting behaviour. So, e.g. oscillating phenomena can evolve - as these oscillations can spread in space via diffusion and instabilities may develop spatial phenomena like pattern formation can be observed and observed. We will see some of the typical examples below.
Furthermore, the analysis and general statements become more difficult; not all properties which are well-known from the scalar case can be directly transferred to systems.

6.2 Conservative systems

Reference: [1]

We start to consider a special kind of reaction-diffusion systems, the so-called conservative systems, which means: the reaction terms are "conservative". Generally, for a conservative system, a function of the dependent variables exists, which is a constant of the motion; it can be interpreted as a kind of "energy". Mathematically formulated:
System $\dot{u} = f(u)$ (m-dimensional) is conservative if a function $G(u)$ exists with

$$\dot{G}(u) = \sum_{i=1}^{m} \frac{\partial G}{\partial u_i} \dot{u}_i = \sum_{i=1}^{m} \frac{\partial G}{\partial u_i} f_i(u) = 0.$$

Of course, such conservative systems have special properties; e.g. they often have oscillatory solutions. Often, they are "easy" to analyse, but from a modelling point of view, there are also disadvantages, as e.g. structural instability (as known from the classical predator-prey model).

6.2.1 Lotka-Volterra system

Nevertheless, we consider here the classical predator-prey model; let's start with the non-dimensionalised version

$$\dot{u} = u(1-v) \tag{6.1}$$
$$\dot{v} = av(u-1) \tag{6.2}$$

Already known: stationary points are $(0,0)$ (saddle-point; via linearisation), $(1,1)$ (centre in the linearised system, but as Hartman-Grobman is not applicable in that case, additional analysis needed). System (6.1), (6.2) can be separated for the variables, i.e. first we get

$$av(u-1)\,du = u(1-v)\,dv,$$

then

$$a\frac{u-1}{u}\,du = \frac{v-1}{v}\,dv,$$

which can be integrated and yields

$$G(u,v) = a(u - \ln u) + v - \ln v = A(const.)$$

This is already known (also that solutions curves are contained in level sets of $G(u,v)$, and can be interpreted in this context as "the quantity $G(u,v)$ is conserved", thus the Lotka-Volterra system is conservative.
A first interesting question concerns small perturbations of the system and how they influence the behaviour of such a system. E.g. if we like to introduce a self-limitation of the prey population, the system looks as follows:

$$\begin{aligned} \dot{u} &= u(1-v)\varepsilon u^2 \\ \dot{v} &= av(u-1) \end{aligned}$$

Even though ε can be assumed very small, there is a significant effect on the behaviour of the system: the coexistence point (now $(1, 1-\varepsilon)$ becomes a stable spiral, and $V(u,v) = a(u - \ln u) + v - (1-\varepsilon)$ a global Lyapunov function, no periodic solutions present anymore. From a biological point of view this means: even a small perturbation could remove the oscillations, which isn't too realistic. From a mathematical point of view, such a behaviour is called "structural instability". Remark, that all conservative systems are structurally unstable. Nevertheless they are interesting to consider as they may teach us about the influences of simple interactions.
Next we consider the Lotka-Volterra system including diffusion for both species (with equal diffusion coefficients) and find some information about the long time behaviour of the solution.

Theorem 17 (Murray, 1975) *The diffusional Lotka-Volterra system,*

$$\begin{aligned} u_t &= u(1-v) + D\Delta u \\ v_t &= av(u-1) + D\Delta u \end{aligned}$$

with equal diffusion coefficients and homogeneous Neumann boundary conditions

$$\frac{\partial u}{\partial n}(x,t) = 0 = \frac{\partial v}{\partial n}(x,t) \qquad on\ x \in \partial\Omega$$

(n the outward normal; Ω bounded subset of $\mathbb{R}^n$) tends to a spatially uniform state for $t \to \infty$.

Proof: Let the initial conditions be

$$u(x,0) = u_0(x), \qquad v(x,0) = v_0(x) \qquad \text{for } x \in \Omega.$$

We define $s(x,t)$, corresponding to the "energy" of the system without diffusion,

$$s = a(u - \ln u) + v - \ln v, \tag{6.3}$$

i.e. for $D = 0$ it satisfies $s_t = 0$. Question: How does the corresponding differential equation for s look like for $D \neq 0$?
We take (6.3) and differentiate it:

$$\begin{aligned} s_t &= a\left(u_t - \frac{u_t}{u}\right) + v_t - \frac{v_t}{v} \\ \Delta s &= a\left(\Delta u - \frac{\Delta u}{u} + \frac{|\nabla u|^2}{u^2}\right) + \Delta v - \frac{\Delta v}{v} + \frac{|\nabla v|^2}{v^2}, \end{aligned}$$

this yields

$$\begin{aligned} s_t - D\Delta s &= a(u_t - D\Delta u)\frac{u-1}{u} + (v_t - D\Delta v)\frac{v-1}{v} - aD|\nabla u|^2/u^2 - D|\nabla v|^2/v^2 \\ &= -aD|\nabla u|^2/u^2 - D|\nabla v|^2/v^2 \leq 0. \end{aligned}$$

using the system equations. This can be interpreted in such a way that the energy is dissipated by the diffusion terms.
The boundary conditions for s are

$$\frac{\partial s}{\partial n}(x,t) = 0 \qquad \text{for } x \in \partial\Omega$$

and the initial condition reads

$$s(x,0) = a(u_0 - \ln u_0) + v_0 - \ln v_0 = s_0(x).$$

(Both follow directly from the conditions for u and v) Via integration over Ω we can define the "total amount of energy" in the system at time t:

$$S(t) = \int_\Omega s(x,t)\,dx.$$

Using the Neumann boundary condition and Green formula yields

$$\begin{aligned}\dot{S}(t) &= \underbrace{\int_\Omega D\Delta s\,dx}_{=D\int_{\partial\Omega}\frac{\partial S}{\partial n}\,ds=0} + \int_\Omega -aD\frac{|\nabla u|^2}{u^2} - D\frac{|\nabla v|^2}{v^2}\,dx \\ &= -D\int_\Omega \frac{a|\nabla u|^2}{u^2} + \frac{|\nabla v|^2}{v^2}\,dx.\end{aligned}$$

Obviously, S is monotone non-increasing; there are two possibilities: it tends to a finite limit or it tends to $-\infty$ for $t \to \infty$. By definition, s satisfies $s(x,t) \geq a+1$, from which we get directly

$$S(t) = \int_\Omega s(x,t)\,dx \geq (a+1)|\Omega|,$$

so S indeed tends to a finite limit, which requires

$$\dot{S} = -D\int_\Omega \frac{a|\nabla u|^2}{u^2} + \frac{|\nabla v|^2}{v^2}\,dx \to 0.$$

The only possibility to satisfy this, is that also ∇u and ∇v tend to 0 for $t \to \infty$, i.e. the system tends to a spatially uniform state.

□

Remark: The result can be also generalised to the case of two differential diffusion coefficients.

What does this theorem mean? The Lotka-Volterra system, even if including diffusion, cannot yield ecological patchiness; no spatial distribution of species in a environment in possible in the long time run.

6.3 Some more basics for Reaction-diffusion systems

Reference: [1]

We learnt already much about properties and useful theorems for (mainly scalar) reaction diffusion equations. Some results can be extended to reaction-diffusion systems, but one has to be careful about the assumptions, and some statements are weaker.

Remark: In the following, order relations, operators like max, min, sup, inf and also the typical properties of solutions and inequalities are defined and interpreted component wise.
To be able to formulate the results in a quite general way, we use the following definition for the boundary conditions:

Definition 9 (Boundary operator) *The boundary operator B is defined by*

$$(Bu)_i = c_i(x,t)u_i(x,t) + d_i(x,t)\frac{\partial u_i}{\partial \nu_i}(x,t),$$

where $(Bu)_i$ denotes component i of the vector Bu, $c_i \geq 0$, $d_i \geq 0$, $c_i^2 + d_1^2 > 0$ and $\frac{\partial}{\partial \nu_i}$ denotes any outward derivative. Remark: B is a diagonal operator, i.e. $(Bu)_i$ only depends on component i of u.

Now we can introduce an invariant set:

Definition 10 (Invariant set) *An invariant set of the (spatially homogeneous) system $u_t = f(u)$ is a set $\Sigma \subset \mathbb{R}^m$ (m dimension of u), such that if u is a solution of $u_t = f(u)$ in $0 < t < T$ for an $T \leq \infty$ with initial conditions $u(0) \in \Sigma$, then the solution stays in Σ, i.e. $u(t) \in \Sigma$ for $0 \leq t \leq T$. In the same way, an invariant set for the initial boundary value problem is a set $\Sigma \subset \mathbb{R}^m$ such that if u is a solution of*

$$u_t = f(u) + \Delta u \qquad in\ \Omega \times (0,T)$$

with all initial and boundary values in Σ, then also $u(x,t) \in \Sigma$ is satisfied for all $x \in \Omega$ and $0 \leq t < T$.

Next, monotonicity is generalised for the higher-dimensional case:

Definition 11 *A function $f(u)$ is called quasi-monotone nondecreasing, if each component $f_i(u)$ is non-decreasing in u_j for each $j \neq i$.*
$f(u)$ is called to possess the mixed quasi-monotone property, if each component $f_i(u)$ is monotone in u_j for each $j \neq i$.

In the following, we consider system which can be written in the following form:

$$\begin{aligned} Nu = Lu - f(u) &= u_t - D\Delta u - f(u) = 0 \qquad \text{in } \Omega \times (0,T] && (6.4)\\ u(x,0) &= u_o(x) \qquad \text{on } \Omega \times \{0\} && (6.5)\\ Bu &= b(x,t) \qquad \text{on } \partial\Omega \times (0,T) && (6.6) \end{aligned}$$

Additional requirements:

- D is the so-called diagonal diffusion matrix (not all entries of the diagonal should be $= 0$)
- B is a diagonal boundary operator

This system (6.4)-(6.6) is called "problem (P)" in this section. The comparison theorem can also be generalised for systems and formulated in the following way:

Theorem 18 (Comparison theorem) *Let the following assumptions hold:*

(i) $\underline{u}$ *and* $\bar{u}$ *are sub- resp. supersolutions of problem (P)*

(ii) f *is uniformly Lipschitz continuous in u*

(iii) $\Omega \times (0,T)$ *satisfies the so-called "interior sphere property" (except for we deal with the Dirichlet problem); this means: a closed ball exists, which is contained in $\Omega \times (0,T)$ and only intersects the boundary at one single point*

(iv) f *is quasi-monotone non-decreasing*

Then it is (according to the weak comparison theorem):

$$\underline{u} \leq \bar{u} \qquad in\ \bar{\Omega} \times [0,T]$$

The strong comparison theorem yields:
For each i one of the two following possibilities holds:

(a) $\underline{u_i} < \bar{u}_i$ *in* $\Omega \times (0,T]$

(b) $\underline{u_i} = \bar{u}_i$ *in* $\Omega \times (0,t^*]$ *for a* $t^* \leq T$.

Rough idea of the proof: The scalar maximum principle is applied to the function $w_i = \bar{u}_i - \underline{u}_i + y$, by that one can show that $w_i > 0$, where y (also a function) depends on a parameter ε and $y \to 0$ for $\varepsilon \to 0$. For the necessary estimates, Lipschitz continuity and the restrictions for f are used. For the strong comparison theorem, the scalar strong maximum principle is applied.

$(\square)$

Remark that the possible interactions of the components via the reaction term f lead to these restrictions for f.

The following corollary gives information about invariant sets:

Corollary 2 *Let assumptions (ii)-(iv) of Theorem 18 hold. Let a, b be constant vectors satisfying $-\infty \leq a \leq b \leq \infty$ and $f(a) \geq 0$, $f(b) \leq 0$. Then $\Sigma = \{u | a \leq u \leq b\}$ is an invariant set for problem (P).*

With these assumptions, it is quite easy to show global existence of a solution!

Theorem 19 (Global existence) *Let assumptions (ii)-(iv) of Theorem 18 hold. If there exists an invariant set $\Sigma = \{u | a \leq u \leq b\}$ for problem (P), then Problem (P) has a solution for all times.*

Proof: Let K be the Lipschitz constant for the reaction function f. Let L_i denote the differential operator for component i, i.e.

$$L_i v_i = \frac{\partial v_i}{\partial t} - D_i \Delta v_i$$

Two sequences $\{v^n\}$ and $\{w^n\}$ are defined in the following way:

$$\begin{aligned} v^0 &= a, \qquad (L_i + K) v_i^n = f_i(v^{n-1}) + K v_i^{n-1} \\ w^0 &= b, \qquad (L_i + K) w_i^n = f_i(w^{n-1}) + K w_i^{n-1} \end{aligned}$$

with the boundary and initial conditions (6.5) and (6.6). It is necessary that aA and b are finite!
To show: $v^{n+1} - v^n \geq 0$ by induction
Start $n = 0$: There we find

$$\begin{aligned} (L_i + K)(v_i^1 - v_i^0) &= f_i(v^0) + K v_i^0 - L_i v_i^0 - K v_i^0 \\ &= -(\underbrace{L_i v_i^0}_{=0} - f_i(v^0)) = f_i(a) \geq 0. \end{aligned}$$

The scalar maximum principle yields $v_i^1 - v_i^0 \geq 0$ (as the initial and boundary conditions have to be satisfied by both).
Induction step: Assume that the statement is already shown for $n-1$. We get

$$\begin{aligned} (L_i + K)(v_i^{n+1} - v_i^n) &= f_i(v^n) + K v_i^n - f_i(v^{n-1}) - K v_i^{n-1} \\ &\geq -K(v_i^n - v_i^{n-1}) + K(v_i^n - v_i^{n-1}) = 0 \end{aligned}$$

(this is valid since f is Lipschitz continuous and quasi-monotone non-decreasing). Applying again the scalar maximum principle yields $v^{n+1} - v_i^n \geq 0$ as desired.
Similarly, for w^n can be shown: $w^{n+1} - w^n \leq 0$.
Now we have a monotonic increasing $\{v^n\}$ and a monotonic decreasing $\{w^n\}$, the limits $v = \lim_{n\to\infty} v^n$ and $w = \lim_{n\to\infty} w^n$ exists. But as there is only a unique solution of the problem, it is $v = w$.

□

Remark: The required quasi-monotonicity is essential. As an example, we consider:

$$\begin{aligned} u_t &= u + u_{xx} \\ v_t &= -u + v + v_{xx} \end{aligned}$$

in the area $(x_1, x_2) \times (0, \infty)$, with the initial conditions $u = u_0$, $v = v_0$ (both constant) and homogeneous Neumann boundary conditions $u_x = v_x = 0$. The solution can be explicitely written as

$$\begin{aligned} u &= u_0 e^t \\ v &= -u_0 t e^t + v_0 e^t \end{aligned}$$

Obviously, if we increase u_0 (the initial condition), u is increased, but v is decreased - "impossible" for the comparison theorem.

For the next step, we introduce another problem, called ($\underline{\text{P}}$), defined similar to problem (P), but with a reaction term $\underline{\text{f}}$ instead of f, which satisfies $\underline{\text{f}}(v) \leq f(v)$. In the same way we can introduce a problem ($\bar{P}$) with a super-reaction function $\bar{f}$.

Corollary 3 *Let $\underline{f} : \mathbb{R}^m \to \mathbb{R}^m$ be a quasi-monotone non-decreasing uniformly Lipschitz continuous function which satisfies $\underline{f}(v) \leq f(v)$ for all $v \in \mathbb{R}^m$. Let $\underline{u}$ be a subsolution of ($\underline{P}$) and let u be a supersolution of (P). Then it is*

$$\underline{u} \leq u \qquad \text{in } \bar{\Omega} \times [0, T]$$

Proof: According to the assumptions, u is a supersolution of (P), hence it is

$$Lu \geq f(u) \geq \underline{f}(u),$$

and then u is a supersolution of ($\underline{\mathrm{P}}$). The function $\underline{f}$ has the monotonicity properties; so one can compare $\underline{u}$ and u and gets $\underline{u} \leq u$.

□

Remark: f itself does not need to have the monotonicity properties. So this is an advantage, compared to the situation before.

Next question: How to find such a quasi-monotone bounding function $\underline{f}$? The following lemma yields a possibility, using an infimum:

Lemma 6 *$\underline{f}$ is defined as follows:*

$$\underline{f}_i(u) = \inf_{\{v | u \leq v \leq \bar{u}, v_i = u_i\}} f_i(v),$$

where $\bar{u}$ is a supersolution (can be chosen). Then it is: $f(u) \geq \underline{f}(u)$ for all u, the newly constructed $\underline{f}$ is quasi-monotone non-decreasing, and it is uniformly Lipschitz continuous, if f is Lipschitz continuous (with the same Lipschitz constant).

(without proof here)

Remark: In the same way one can construct $\bar{f}$ by

$$\bar{f}_i(u) = \sup_{\{v | \underline{u} \leq v \leq u, v_i = u_i\}} f_i(v)$$

for a subsolution $\underline{u}$.

The next theorem (where we omit again the proof; it contains several sub- and supersolutions, and the Lipschitz continuity for some estimates) gives a good possibility to get an invariant set; here the so-called invariant rectangles:

Theorem 20 (Invariant Rectangles) *Let f be Lipschitz continuous, and $\Omega \times (0,T)$ satisfy the interior sphere property (unless the Dirichlet problem is considered). If $-\infty < a < b < \infty$ are two constant vectors in $\mathbb{R}^m$ such that*

$$\begin{aligned} f_i(v) \geq 0 \qquad & \text{for } v_i = a_i, \quad a \leq v \leq b \\ f_i(v) \leq 0 \qquad & \text{for } v_i = b_i, \quad a \leq v \leq b, \end{aligned}$$

then $\Sigma = \{v | a \leq v \leq b\} \subset \mathbb{R}^m$ is an invariant set for problem (P).

It is even possible to find a global solution with these assumptions:

Theorem 21 (Global existence) *Let the assumptions for Theorem 20 be satisfied. Then problem (P) with initial conditions and boundary conditions which are in Σ has a unique global solution.*

Proof: not shown here.

These theorems can be useful to show existence of solutions and even find bounds for the solution.

Example: A competition model for two species (Volterra) including diffusion for both species (the nondimensionalised version):

$$\frac{\partial u_1}{\partial t} = u_1(1 - u_1 - \alpha u_2) + D_1 \Delta u_1 = f_1(u_1, u_2) + D_1 \Delta u_1 \tag{6.7}$$

$$\frac{\partial u_2}{\partial t} = \theta u_2(1 - \beta u_1 - u_2) + D_2 \Delta u_2 = f_2(u_1, u_2) + D_2 \Delta u_2 \tag{6.8}$$

in $\Omega \times (0,T]$. homogeneous Neumann boundary conditions

$$\frac{\partial u_1}{\partial n}(x,t) = 0 = \frac{\partial u_2}{\partial n}(x,t) \qquad \text{on } \partial\Omega \tag{6.9}$$

and initial conditions

$$u_1(x,0) = u_{1,0}(x), \qquad u_2(x,0) = u_{2,0}(x) \qquad \text{on } \Omega \times \{0\}. \tag{6.10}$$

Theorem 22 *Let the initial data (6.10) be nonnegative and bounded, i.e.*

$$0 \leq (u_{1,0}, u_{2,0}) \leq M = (M_1, M_2),$$

then the competition model with diffusion (6.7),(6.8) with homogeneous Neumann boundary conditions (6.9) has solutions which satisfy

$$0 \leq (u_1, u_2) \leq b = (b_1, b_2),$$

where $b_1 = \max(N_1, 1)$. $b_2 = \max(M_2, 1)$.

Proof: The given $a = 0$ and b satisfy the required conditions for f in Theorem 20, the invariant rectangles:

$$\begin{aligned} f_1(a_1, u_2) = 0 &\geq 0 && \text{for } a_1 = 0 \\ f_2(u_1, a_2) = 0 &\geq 0 && \text{for } a_2 = 0 \\ f_1(b_1, u_2) = b_1(1 - b_1 - \alpha u_2) &\geq 0 && \text{since } b_1 \geq 1 \\ f_2(u_1, b_2) = \theta b_2(1 - \beta u_1 - b_2) &\leq 0 && \text{since } b_2 \geq 1. \end{aligned}$$

The boundary conditions and the initial conditions also satisfy the requirements, (for the boundary conditions, we have $\frac{\partial a}{\partial n} = \frac{\partial u}{\partial n} = \frac{\partial b}{\partial n} = 0$)
so indeed $\Sigma = \{v | a \leq v \leq b\} \subset \mathbb{R}^2$ is an invariant set for the given competition model.

□

Chapter 7

Waves

7.1 Plane waves

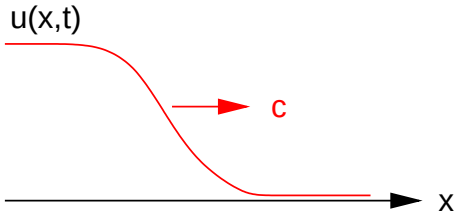
7.1.1 Introduction

Literature: [4, 11]

Typical question: Is it possible for a species to invade into new habitats and how does this work?

Approach: Travelling wave solutions of a reaction-diffusion equation.

The goal is to find solutions of the following form,



which can describe such an invasion into a new habitat, where this move appears with a constant speed c (the so-called wave speed), i.e.

$$u(x,t) = \phi(x - ct).$$

The new variable $z := x - ct$ denotes the wave variable and $\phi(z)$ is the wave profile. The travelling wave ansatz includes conditions at $\pm\infty$ instead of "classical" boundary conditions:

$$u(x,t) = \phi(x - ct), \quad \phi(-\infty) = 1, \quad \phi(+\infty) = 0, \tag{7.1}$$

which means that the population has reached its capacity for $x \to -\infty$ (normalised to 1), and no population has arrived yet for $x \to +\infty$. (7.1) leads to:

$$\frac{\partial}{\partial t}u(x,t) = -c\phi', \quad \frac{\partial^2}{\partial x^2}u(x,t) = \phi''.$$

As an example for a reaction-diffusion equation, we take here again the Fisher equation

$$u_t = Du_{xx} + \mu u(1-u);$$

together with the travelling wave ansatz, this yields

$$-c\phi' = D\phi'' + \mu\phi(1-\phi),$$

which corresponds to a second order ODE and we can transform it into a 2D system of first order ODEs by introducing a new variable $v := \phi'$; we write again u instead of ϕ for reasons of simplicity:

$$\begin{aligned} u' &= v \\ v' &= -\frac{c}{D}v - \frac{\mu}{D}u(1-u). \end{aligned} \tag{7.2}$$

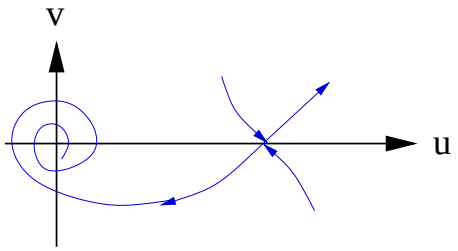
The stationary states here are $P_1 = (0,0)$ and $P_2 = (1,0)$. The general Jacobian reads

$$J = \begin{pmatrix} 0 & 1 \\ -\frac{\mu}{D} + 2\frac{\mu}{D}u & -\frac{c}{D} \end{pmatrix}.$$

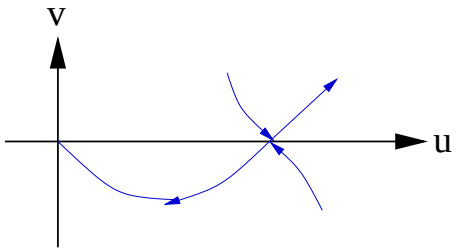
Applied on the stationary states, we get

- $J(0,0) = \begin{pmatrix} 0 & 1 \\ -\frac{\mu}{D} & -\frac{c}{D} \end{pmatrix}$, i.e. $det = \frac{\mu}{D} > 0$ and $tr = -\frac{c}{D}$, so at least, $(0,0)$ is stable. The discriminant is $tr^2 - 4det = \frac{c^2}{D^2} - 4\frac{\mu}{D}$, thus, for $c < 2\sqrt{D\mu}$ we have a stable spiral and for $c > 2\sqrt{D\mu}$ a stable node.
- $J(1,0) = \begin{pmatrix} 0 & 1 \\ \frac{\mu}{D} & -\frac{c}{D} \end{pmatrix}$, i.e. $det = -\frac{\mu}{D} < 0$, so, there is always a saddle in $(1,0)$.

For the wave profile, we need $u(-\infty) = 1$ and $u(+\infty) = 0$, and also $v(-\infty) = v(+\infty) = 0$. Considering the phase portrait of (7.2), we are looking for a connection from the stationary point $(1,0)$ to $(0,0)$. Since u describes a population density, negative values are not biologically meaningful. In the case of $c < 2\sqrt{D\mu}$, $(0,0)$ is a stable spiral:

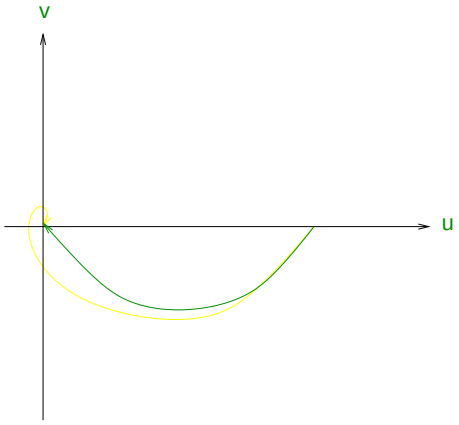


obviously leading to negative values for u (this case corresponds to a so-called oscillating front). So, $c^* = 2\sqrt{D\mu}$ is the minimal wave speed for the existence of a wavefront solution; for $c > c^*$, $(0,0)$ is a stable node.

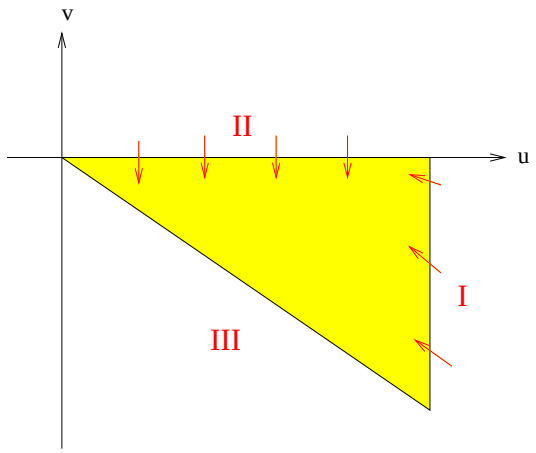


A proof can be found in [8].

Until now, we only know that $c \geq 2\sqrt{D\mu}$ is necessary, we do not now, if it is also a sufficient condition. But, indeed, using the properties of the vector field shows that the solution curve which leaves the saddle point $(1,0)$ ends up in the stable node $(0,0)$. This corresponds to the heteroclinic orbit for what we are looking.
In the following, we use $D = 1$ and $\mu = 1$, just for simplicity of notation. Sketch of the phase plane and the heteroclinic orbit:



(Remark: the yellow curve shows the behaviour in case of $c < 2$, with the stable focus in $(0, 0)$, as already shown above)
We introduce a triangular region in the (u, v) phase plane in the following way:



I.e. the sides are defined as follows:

(I) $u = 1$, $v < 0$

(II) $v = 0$, $0 < u < 1$

(III) $v = -\alpha u$, $0 < u < 1$

In case of $c \geq 2$, the unstable manifold (i,e. the eigenvector corresponding to the positive eigenvalue) of the saddle point at $(1, 0)$ points into the triangular region.
Next we check, how the vector field behaves on the sides:

On (I): There we have

$$\begin{aligned} u' = v &< 0 \\ v' = -cv &> 0, \end{aligned}$$

i.e. the arrows point into the triangular region.

On (II): There we have

$$\begin{aligned} u' &= 0 \\ v' = -u(1-u) &< 0, \end{aligned}$$

i.e. the arrows point into the triangular region.

On (III): There we consider the scalar product between the vector field and the normal vector (pointing into the triangular region) in III:

$$\begin{aligned} \begin{pmatrix} v \\ -cv - u(1-u) \end{pmatrix} \cdot \begin{pmatrix} \alpha \\ 1 \end{pmatrix} &= \alpha v - cv - u(1-u) \\ &= -\alpha^2 u + \alpha c u - u(1-u) \\ &= -u(\alpha^2 - c\alpha + (1-u)) \end{aligned}$$

using $v = -\alpha u$ for the second step, as we are on III. In order to have arrows of the vector field which point into the triangular region, the scalar product should be positive. We still can choose α, this is the big chance now: We need

$$\alpha^2 - c\alpha + 1 - u < 0.$$

Due to the assumptions, we have $0 < u < 1$, hence

$$\alpha^2 - c\alpha + 1 - u < \alpha^2 - c\alpha + 1.$$

So, it is sufficient to choose an α which satisfies

$$\alpha^2 - c\alpha + 1 \leq 0,$$

a parabola. To be able to find a positive α which satisfies this inequality, a parabola with two positive real roots is useful. The roots of the parabola are

$$\alpha = \frac{c \pm \sqrt{c^2 - 4}}{2},$$

they are positive and real for $c \geq 2$. With these restrictions, we can choose an α, such that the vector fields points into the triangular region, also through III.
What happens with the unstable manifold of the saddle point (1,0)? It enters the triangular region and cannot leave it. There is no stationary point in the interior of the triangular region. A closed orbit can also be excluded, via the negative criterion of Bendixson-Dulac, as we find

$$\text{div } (u, v) = \frac{\partial v}{\partial u} + \frac{\partial(-cv - u(1-u))}{\partial v} = -c \neq 0.$$

The only chance is to tend to $(0, 0)$ which corresponds to the heteroclinic orbit, i.e. the travelling wave solution.

Remark 3 *For linear parabolic equations like the standard diffusion equation, there are no physically realistic travelling wave solutions; for that purpose it is necessary to "add" a nonlinear term; e.g. the considered reaction-diffusion equations can exhibit such solutions. Of course, their form depends on the additional term $f(u)$.*

Until now, we derived only a criterion which gives information about the possible wave speeds, but nothing about the appearance of propagation speeds in the reality. E.g. we can consider the dependency of the wavespeed c on the initial conditions at infinity (Reference: [11]): When the leading edge of the evolving wave is considered, of course u is small there. An idea could be to neglect there u^2 compared to u, so the linearised version of the Fisher equation reads

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + u.$$

We use an initial condition which behaves like

$$u(x, 0) \sim Ae^{-ax} \qquad \text{as } x \to \infty,$$

$a > 0$ and $A > 0$ can be chosen arbitrarily. Now we look for travelling wave solutions for the linearised equation of the following form:

$$u(x, t) = Ae^{-a(x-ct)}.$$

This can be interpreted as the leading edge form of the wavefront solution of the nonlinear Fisher equation. Inserting it into the linear equation yields

$$caAe^{-a(x-ct)} = a^2 Ae^{-a(x-ct)} + Ae^{-a(x-ct)},$$

thus there is a relationship between c and a:

$$ca = a^2 + 1 \qquad \rightsquigarrow \qquad c = a + \frac{1}{a}.$$

If c is interpreted as function of a, it assumes its minimum at $a = 1$ with $c_{min} = 2$; for all other $a > 0$, the corresponding wave speed is $c > 2$.
Indeed, the asymptotic wave speed for $0 < a \leq 1$ is $c = a + \frac{1}{a}$.
But for $a > 1$ something different happens: There it is $e^{-ax} < e^{-x}$ (for positive x), thus also

$$u(x, t) = A^{-a(x-ct)} < Ae^{-(x-ct)}$$

According to above, Ae^{x-ct} has the wavespeed $c = 2$, so functions below that cannot spread out faster than the "upper bound". Two cases have to be distinguished:

- $0 < a \leq 1 \Rightarrow c = a + \frac{1}{a}$

- $a \geq 1 \Rightarrow c = 2$

(for more explanation and background see [10])

Next question: How to determine the profile of the travelling wave solution?
From the ODE system we get directly: a solution $v(u)$ satisfies

$$\frac{dv}{du} = \frac{-cv - u(1-u)}{v}, \tag{7.3}$$

thus also the heteroclinic orbit.
Let $v = \frac{1}{c}y$, then we can rewrite equation (7.3):

$$\varepsilon y \frac{dy}{du} = -y + u(u-1), \tag{7.4}$$

where $\varepsilon = \frac{1}{c^2}$. At least we know that ε is not too big (due to $c \geq 2$, so it might make sense to expand y as a power series in ε:

$$y(u, \varepsilon) = y_0(u) + \varepsilon y_1(u) + \varepsilon^2 y_2(u) + \dots$$

This is inserted into (7.4):

$$\begin{aligned} \varepsilon(y_0(u) + \varepsilon y_1(u) + \varepsilon^2 y_2(u) + \dots) \cdot (\frac{dy_0}{du} + \varepsilon \frac{dy_1}{du} + \varepsilon^2 \frac{dy_2}{du} + \dots) \\ = -(y_0(u) + \varepsilon y_1(u) + \varepsilon^2 y_2(u) + \dots) + u(u-1). \end{aligned}$$

We split up that equation into the different orders (i.e. powers) in ε:

ε^0: $y_0(u) = u(u-1)$

ε^1: $y_1(u) = -y_0(u) \cdot \frac{dy_0}{du}$

ε^2: $y_2(u) = -y_1(u) \cdot \frac{dy_0}{du} - y_0(u) \cdot \frac{dy_1}{du}$,

So, the heteroclinic orbit can be written as

$$\begin{aligned} y(u) &= y_0(u) - \varepsilon \underbrace{y_0(u)\frac{dy_0}{du}}_{y_1(u)} - \varepsilon^2 \underbrace{y_1(u)\frac{dy_0}{du} + y_0(u)\frac{dy_1}{du})}_{y_2(u)} \\ &= u(u-1) - \varepsilon u(u-1)(2u-1) + \dots \end{aligned}$$

Of course, this can be written also in the original variables u and v:

$$v(u) = \varepsilon^{1/2}(u^2 - u) - \varepsilon^{3/2}(2u^3 - 3u^2 + u) + \dots$$

Now, we have a description in variables u and v. But of course, one is interested more in a solution for u dependent e.g. on z. We can use a similar idea:
Let $s = \frac{z}{c}$, then the wave equation (the ODE of 2nd order) is transformed into

$$\varepsilon u'' + u' + u(1-u) = 0. \tag{7.5}$$

Even though the ε appears in the term with the highest derivative, also for $\varepsilon = 0$ both "additional wave conditions" ($u(-\infty) = 1$ and $u(+\infty) = 0$) can be satisfied also for $\varepsilon = 0$, i.e. we really deal with a regular perturbation problem. Now we can expand u in terms (powers) of ε:

$$u(s, \varepsilon) = u_0(s) + \varepsilon u_1(s) + \dots,$$

this is substituted in (7.5), we split up the different powers of ε and get:

ε^0: $u_0' = -u_0(1 - u_0)$

ε^1: $u_1' + (1 - 2u_0)u_1 = -u_0''$

s can be shifted arbitrarily, since the equation (7.5) and the travelling wave solution both are invariant to translations in s. Thus, we choose $s = 0$ as point where $u = 1/2$ for all ε, i.e.

$$\begin{aligned} u_0 &= \frac{1}{2} \\ u_i &= 0 \qquad \text{for } i = 1, 2, 3, \ldots \end{aligned}$$

Hence, we can solve the equations for the single orders in ε step by step and get

$$\begin{aligned} u_0(s) &= \frac{1}{1+e^s} \\ u_1(s) &= \frac{e^s}{(1+e^s)^2} \ln\left(\frac{4e^s}{(1+e^s)^2}\right), \end{aligned}$$

and rewritten in the original variable z:

$$u(z,\varepsilon) = \frac{1}{1+e^{z/c}} + \frac{1}{c^2}\frac{e^{z/c}}{(1+e^{z/c})^2} \ln\left(\frac{4e^{z/c}}{(1+e^{z/c})}^2\right) + \mathcal{O}(c^{-4})$$

Next step: One can also show that the travelling wave solution for the Fisher equation is stable! This is not possible (and true) in general (e.g. not under perturbations in the far field, the limit $|x| \to \infty$), but e.g. for the special case of small perturbations of compact support in the "moving coordinate" from of the wave.
The Fisher equation can be written in the so-called moving coordinate frame; that means: we keep the dependency on t but replace dependency on the spatial variable x by the wave variable $z = x - ct$:

$$\frac{\partial u}{\partial t} = u(1-u) + c\frac{\partial u}{\partial z} + \frac{\partial^2 u}{\partial z^2}, \tag{7.6}$$

i.e. we consider $u(x,t) = u(z,t)$ as the dependent variable.
Let $c \geq 2$, we assume that there exists a travelling wave solution of the form

$$u(z,t) = u_c(z)$$

(c arbitrary). As usual, for checking the stability we introduce a small perturbation $v(z,t)$ to $u_c(z)$:

$$u(z,t) = u_c(z) + v(z,t). \tag{7.7}$$

For this perturbation it is assumed that it vanishes outside a finite interval L (in the moving frame), i.e.

$$v(z,t) = 0 \qquad \text{for } |z| \geq L.$$

Approach (7.7) is inserted into the Fisher equation (in the moving coordinate frame, (7.6)) and yields

$$\begin{aligned} \frac{\partial(u_c(z)+v(z,t))}{\partial t} &= (u_c(z)+v(z,t))(1-u_c(z)-v(z,t)) + c\frac{\partial(u_c(z)+v(z,t))}{\partial z} + \frac{\partial^2(u_c(z)+v(z,t))}{\partial z^2} \\ \Leftrightarrow \qquad \frac{\partial v}{\partial t} &= (1-2u_c(z))v(z,t) - v^2(z,t) + c\frac{\partial v}{\partial z} + \frac{\partial^2 v}{\partial z^2} \end{aligned}$$

(using the fact that $u_c(z)$ is travelling wave solution)
$v(z,t)$, as a perturbation, is assumed to be small, so higher order terms in v can be neglected, resulting in

$$\frac{\partial v}{\partial t} = (1-2u_c(z))v(z,t) + c\frac{\partial v}{\partial z} + \frac{\partial^2 v}{\partial z^2}.$$

We try to find a solution of the following form:

$$v(z,t) = g(z)e^{-\lambda t}$$

Inserting this into the simplified equation yields

$$\begin{aligned} -\lambda e^{-\lambda t}g(z) &= (1-2u_c(z))g(z)e^{-\lambda t} + cg'(z)e^{-\lambda t} + g''(z)e^{-\lambda t} \\ \Leftrightarrow \qquad 0 &= g'' + cg' + (\lambda + 1 - 2u_c(z))g. \end{aligned} \tag{7.8}$$

Idea: We can use the so-called "Liouville-Green transformation", i.e. use the approach

$$g(z) = h(z)e^{-cz/2}.$$

The derivatives thereof are

$$\begin{aligned} g'(z) &= h'(z)e^{-cz/2} - h(z)\frac{c}{2}e^{-cz/2} \\ g''(z) &= h''(z)e^{-cz/2} - h'(z)\frac{c}{2}e^{-cz/2} - h'(z)\frac{c}{2}e^{-cz/2} + h(z)\frac{c^2}{4}e^{-cz/2} \\ &= h''(z)e^{-cz/2} - ch'(z)e^{-cz/2} + h(z)\frac{c^2}{4}e^{-cz/2}. \end{aligned}$$

Insert this into (7.8), then we get:

$$\begin{aligned} 0 &= h''(z)e^{-cz/2} - ch'(z)e^{-cz/2} + h(z)\frac{c^2}{4}e^{-cz/2} \\ &\quad + ch'(z)e^{-cz/2} - h(z)\frac{c^2}{2}e^{-cz/2} + (\lambda + 1 - 2u_c(z))h(z)e^{-cz/2} \qquad (7.9) \\ \Leftrightarrow \quad 0 &= h'' + h(\lambda - q(z)), \qquad (7.10) \end{aligned}$$

where

$$q(z) = 2u_c(z) - 1 + \frac{c^2}{4}.$$

(Remark that the derivative of first order has vanished)
From $v(z,t) = 0$ for $|z| \leq L$ we need j to satisfy

$$h(-L) = 0 = h(+L) \qquad (7.11)$$

(7.10) and (7.11) (similar to homogeneous Dirichlet conditions) form a so-called regular Sturm-Liouville problem. Such a problem has nice properties, e.g. there exists a countable sequence of eigenvalues which diverges to $+\infty$. Furthermore, the lowest eigenfunction can be chosen to be positive.

Goal: Show that all eigenvalues of the problem are positive, then a positive function h can be assumed in each case (if it is not identically zero), otherwise the perturbation couldn't be displayed in the chosen way), but it is $v(z,t) \to 0$ for $t \to 0$ (due to $v(z,t) = h(z)e^{-cz/2}e^{-\lambda t}$), i.e. the travelling wave is asymptotically stable.

Assume that $h(z)$ is an eigenfunction of (7.10) for the eigenvalue λ. We take (7.10), multiply it by $h(z)$ and integrate over z:

$$\int_{-L}^{+L} (h\frac{d^2h}{dz^2} - qh^2)\,dz + \lambda \int_{-L}^{+L} h^2\,dz = 0.$$

Partial integration yields

$$\int_{-L}^{+L} h\frac{d^2h}{dz^2}\,dz = \underbrace{[h(z)h'(z)]_{-L}^{+L}}_{=0} - \int_{-L}^{+L} (h'(z))^2, dz,$$

thus

$$\lambda = \frac{\int_{-L}^{+L}((h'(z))^2 + qh^2)\,dz}{\int_{-L}^{+L} h^2\,dz},$$

the so-called Rayleigh quotient.

Remark that the eigenvalues here are formulated by using the eigenfunctions (for that the knowledge of the eigenvalues would be necessary ...), so it is not useful for an explicit computation. Nevertheless, this formula contains a useful information, as it is

$$q(z) = 2u_c(z) + \frac{c^2}{4} - 1 \geq 2u_c(z) > 0$$

(due to $c \geq 2$). Hence we get all λ's to be positive, as desired; thus the asymptotic stability of the travelling wave solution.

7.1.2 Different types of waves

Reference: [7]

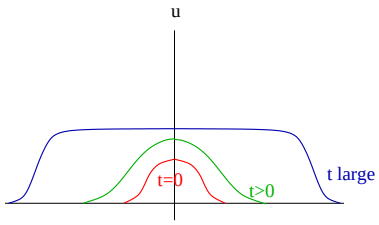
In general, different types of travelling waves can appear, typically:

- Wave trains: the wave profile $V(\xi)$ is periodic
- Wave fronts: $V(-\infty)$ and $V(\infty)$ exist and are unequal
  (as it was the case in our first example with the Fisher equation)
- Pulses: $V(-\infty)$ and $V(\infty)$ exist, are equal, but $V(\xi$ is not constant.

The approach is as usual; but the boundary conditions change.

7.1.3 Radially symmetric wave

Remark that the Fisher equation is invariant under change of sign of x, which means, there is also a wave solution of the form $u(x,t) = \phi(x+ct)$ with the boundary conditions $\phi(-\infty) = 0$ and $\phi(\infty) = 1$.
If we start with an initial conditions $u(x,0)$ which is > 0 in a finite domain and $= 0$ outside that finite domain, two travelling wavefronts will evolve: one to the left and the other to the right! Both wave fronts have speed $c = 2$. Clearly, in case of $u(x,0) < 1$, the logistic growth term causes the travelling wave solution to grow until $u = 1$; so $u(x,t) \to 1$ for $t \to \infty$ for all x.



Question: Is it possible to have a similar behaviour for the radially symmetric case, i.e. consider the radius instead of the cartesian coordinate x?
The Fisher equation reads for the radially symmetric case in polar coordinates:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + u(1-u) \tag{7.12}$$

Using the standard approach $z = r - ct$ doesn't lead to an ordinary differential equation, the term $\frac{1}{r}\frac{\partial u}{\partial r}$ prevents this by the explicit dependency on r.
But we can imagine, what happens: With an initial condition as above, u will of course grow since $u < 1$, due to the logistic growth term. Additionally, diffusion is present, so the solution "spreads" out, somehow wavelike. But on the wave, we have $\frac{\partial u}{\partial r} < 0$, thus the right-hand side of equation (7.12) is reduced, compared to the standard case. Equivalently, one could say that either the diffusion is reduced or the reaction term is reduced, compared to the standard case; resulting in a reduced wave speed. For large r the influence of this term vanishes, so the solution will tend asymptotically to the travelling wavefront solution with speed $c = 2$ in the standard case. In some sense, one could say, that here, the wave speed depends on r, i.e. something like $c(r)$.

7.2 Waves in Reaction-Diffusion systems

Until now, we just considered one species, i.e. a scalar equation in mathematical terms, which spreads in space. Of course, this phenomenon is also interesting for systems of reaction diffusion equations, where e.g. several species interact.
The basic questions are:

- Are travelling waves also possible for systems?
- How to find them?
- Which phenomena may appear?

7.2.1 The spread of rabies

Reference: [9]

Rabies may infect all warm-blooded animals, also birds, and also humans, and affects the central nervous system. Vaccines are available (but expensive); but no further cure is known.
The spread seems to occur in waves, e.g. one coming from the Polish-Russian border; the spread velocity is approx. 30-60 km/year.
Model assumptions: There are two groups of foxes:

- Susceptible foxes (S), with no diffusion (as they are "territorial")
- Infective foxes (I), with diffusion (loss of sense of territory), constant death rate

The infection rate is assumed to be proportional to their densities, no reproduction or further spread:

$$\begin{aligned} \frac{\partial S}{\partial t} &= -rIS \\ \frac{\partial I}{\partial t} &= rIS - aI + D\frac{\partial^2 I}{\partial x^2}, \end{aligned}$$

respectively the non-dimensionalised version

$$\begin{aligned} \frac{\partial S}{\partial t} &= -SI \\ \frac{\partial I}{\partial t} &= SI - mI + \frac{\partial^2 I}{\partial x^2}, \end{aligned}$$

where $m = \frac{a}{rS_0}$.
Now we look for a travelling wave solution of this system of the form

$$\begin{aligned} S(x,t) &= S(x-ct) = S(z) \\ I(x,t) &= I(x-ct) = I(z). \end{aligned}$$

This approach yields two ODEs:

$$\begin{aligned} -cS' &= -IS \\ -cI' &= SI - mI + I'' \end{aligned}$$

or equivalently

$$cS' = IS \tag{7.13}$$

$$I'' + cI' + (S-m)I = 0. \tag{7.14}$$

For the boundary conditions, we assume that "far away", there are no infectious foxes, i.e.

$$S(+\infty) = 1, \qquad I(+\infty) = 0.$$

After the wave, again no infectives are assumed (since rabies are fatal in nearly all cases); the number of susceptibles is unknown, but constant, i.e.

$$S'(-\infty) = 0, \qquad I(-\infty) = 0.$$

Inserting (7.13) into (7.14) yields

$$I'' + cI' + \frac{cS'(S-m)}{S} = 0.$$

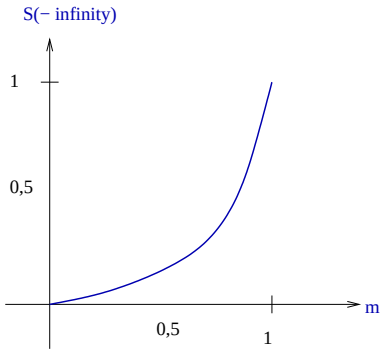
This equation can be integrated:

$$I' + cI + cS - cm\ln S = const. \tag{7.15}$$

For the constant on the right hand side, remark that $S(+\infty) = 1$ and $I(+\infty) = 0$ have to be satisfied, then $const. = c$ has to be chosen.
From the boundary condition at $z = -\infty$ it follows that

$$cS(-\infty) - cm\ln S(-\infty) = c \qquad \Leftrightarrow \qquad \frac{S(-\infty)-1}{\ln S(-\infty)} = m = \frac{a}{rS_o}.$$

So, we can (in principle) determine the fraction of susceptibles, which survives the "rabies wave". The graph looks roughly as follows:



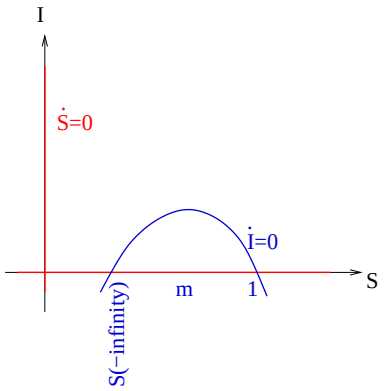
The condition $m < 1$ has to be satisfied for allowing for an epidemic wave; for $m > 1 \Leftrightarrow a > rS_o$ the mortality rate is higher than the recruitment rate for new infectives, which leads to a "die-out" of the rabies. Thus, the critical density for susceptible foxes (for $m = 1$) is $S_0 = \frac{a}{r}$.
We continue by considering the system (7.13), (7.15):

$$\begin{aligned} S' &= \frac{1}{c} IS \\ I' &= -c(S + I) + mc \ln S + c. \end{aligned}$$

Standard analysis yields:

$$\begin{aligned} \dot{S} = 0 &\Leftrightarrow S = 0 \text{ or } I = 0 \\ \dot{I} = 0 &\Leftrightarrow I = m \ln S - S + 1 \end{aligned}$$

Phase plane:



There are two interesting equilibria: $(S(-\infty), 0)$ and $(1, 0)$.
The general Jacobian matrix reads

$$J = \begin{pmatrix} \frac{I}{c} & \frac{S}{c} \\ -c + \frac{mc}{S} & -c \end{pmatrix}.$$

In $(S(-\infty), 0)$:

$$J = \begin{pmatrix} 0 & \frac{S(-\infty)}{c} \\ -c + \frac{mc}{S(-\infty)} & -c \end{pmatrix}$$

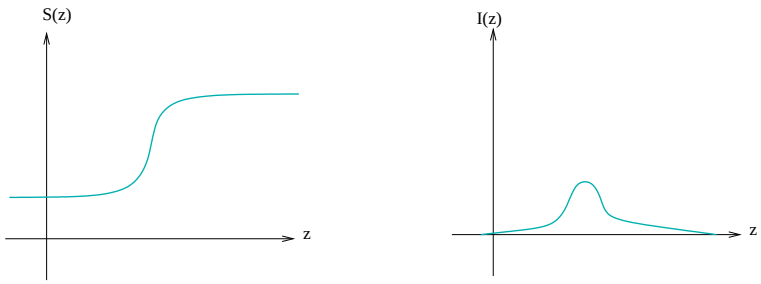
with the determinant $det = +S(-\infty) - m < 0$, hence $(S(-\infty), 0)$ is a saddle point.
In $(1, 0)$:

$$J = \begin{pmatrix} 0 & \frac{1}{c} \\ c(m-1) & -c \end{pmatrix}$$

with the characteristic polynomial $\lambda^2 + c\lambda + (1 - m) = 0$ and the eigenvalues

$$\lambda = \frac{-c \pm \sqrt{c^2 - 4(1-m)}}{2}$$

We can see: For $c < 2\sqrt{1-m}$, $(1, 0)$ is a stable spiral, it is impossible to have a positive heteroclinic connection to $(S(-\infty), 0)$. But for $c \geq 2\sqrt{1-m}$, $(1, 0)$ is a stable node and this connection is possible. Hence, $c = 2\sqrt{1-m}$ corresponds to the minimum wave speed.
From the phaseplane, we can observe roughly the shape of the travelling wave



The susceptible population is monotone decreasing, whereas the infective population shows up a peak.

Remark: In observations in nature, oscillations in the susceptibles and the infectious populations can be found, caused by population dynamics (and not reflected by our model). Such a model system could look like

$$\begin{aligned} \frac{\partial S}{\partial t} &= -rIS + BS(1 - \frac{S}{S_0}) \\ \frac{\partial I}{\partial t} &= rIS - aI + D\frac{\partial^2 I}{\partial x^2} \end{aligned}$$

$\rightsquigarrow$ see exercises

7.2.2 Waves of pursuit and evasion in predator-prey systems

Reference: [12]

Question: Is it possible that travelling wavefronts in a predator-prey system occur? In nature, phenomena of this type can be observed, e.g. travelling bands of oceanic plankton.
Here we deal just with the basic ideas, find conditions which allow for such spatial waves without really "proving" the existence.

We consider a simple predator-prey model with logistic growth of the prey; both species "diffuse" (U: prey, V: predator):

$$\frac{\partial U}{\partial t} = AU\left(1 - \frac{U}{K}\right) - BUV + D_1 \Delta U \tag{7.16}$$

$$\frac{\partial V}{\partial t} = CUV - DV + D_2 \Delta V \tag{7.17}$$

This system can be nondimensionalised by choosing

$$u = \frac{U}{K}, \quad v = \frac{BV}{A}, \quad t^* = At, \quad x^* = x\left(\frac{A}{D_2}\right)^{1/2}$$

$$D^* = \frac{D_1}{D_2}, \quad a = \frac{CK}{A}, \quad b = \frac{D}{CK}$$

(the asterisks are left out in the following, for a simpler notation), so we get (considering only the 1D case):

$$\frac{\partial u}{\partial t} = u(1 - u - v) + D\frac{\partial^2 u}{\partial x^2} \tag{7.18}$$

$$\frac{\partial v}{\partial t} = av(u - b) + \frac{\partial^2 v}{\partial x^2} \tag{7.19}$$

For the spatially independent system, we know already that there exist three stationary points: $(0, 0)$, $(1, 0)$ and $(b, 1 - b)$; using a Lyapunov function one can show that the coexistence point is globally stable (for $b < 1$ of course).

Next, we look for travelling wave solutions (in this example travelling to the left), with the wave variable $z = x + ct$:

$$u(x, t) = U(z), \qquad v(x, t) = V(z).$$

With the typical substitution we get:

$$\begin{aligned} cU' &= U(1-U-V)+DU'' \\ cV' &= aV(U-b)+V'' \end{aligned}$$

In general, we would need to analyse a 4D ODE system of first order now. As a simpler case, we assume that the prey is diffusing much slower than the predators (e.g. consider a system, where animals eat some plants), thus $D=0$ is assumed. So we get a 3D ODE system of first order:

$$\begin{aligned} U' &= \frac{1}{c}U(1-U-V) \\ V' &= W \\ W' &= cW - aV(U-b) \end{aligned}$$

The basic idea is: Try to find heteroclinic connections between stationary points, which correspond to travelling waves.
The stationary points of this system are:

$$(0,0,0), \qquad (1,0,0) \qquad \text{and} \qquad (b,1-b,0)$$

General Jacobian matrix:

$$\begin{pmatrix} \frac{1}{c}-\frac{2}{c}U-\frac{1}{c}V & -\frac{1}{c}U & 0 \\ 0 & 0 & 1 \\ -aV & -a(U-b) & c \end{pmatrix}$$

We cannot use the "zoo" for 2D systems, nevertheless, the signs of the (real parts of the) eigenvalues yield information concerning stability.
Jacobian matrix in $(1,0,0)$:

$$\begin{pmatrix} -\frac{1}{c} & -\frac{1}{c} & 0 \\ 0 & 0 & 1 \\ 0 & -a(1-b) & c \end{pmatrix},$$

the eigenvalues can be computed to be

$$\lambda_1 = -\frac{1}{c}, \qquad \lambda_{2,3} = \frac{1}{2}(c+\sqrt{c^2-4a(1-b)}).$$

For $c>0$, $\lambda_{2,3}>0$, thus an unstable manifold exists. $(1,0,0)$ is oscillatory unstable if $c^2<4a(1-b)$. Hence we need

$$c \geq \sqrt{4a(1-b)}, \qquad b<1$$

for keeping the possibility of a travelling wavefront.
Jacobian matrix in $(0,0,0)$:

$$\begin{pmatrix} \frac{1}{c} & 0 & 0 \\ 0 & 0 & 1 \\ 0 & ab & c \end{pmatrix},$$

the eigenvalues can be computed to be

$$0 = det \begin{pmatrix} \frac{1}{c}-\lambda & 0 & 0 \\ 0 & -\lambda & 1 \\ 0 & ab & c-\lambda \end{pmatrix} = (\frac{1}{c}-\lambda)(\lambda(\lambda-c)-ab),$$

thus

$$\lambda_1 = \frac{1}{c}, \qquad \lambda_{2,3} = \frac{c \pm \sqrt{c^2+4ab}}{2},$$

$\rightsquigarrow (0,0,0)$ is unstable.
Jacobian matrix in $(b,1-b,0)$:

$$\begin{pmatrix} \frac{1}{c}-\frac{2b}{c}-\frac{1-b}{c} & -\frac{b}{c} & 0 \\ 0 & 0 & 1 \\ -a(1-b) & 0 & c \end{pmatrix},$$

the eigenvalues can be computed to be

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

with the cubic characteristic polynomial

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

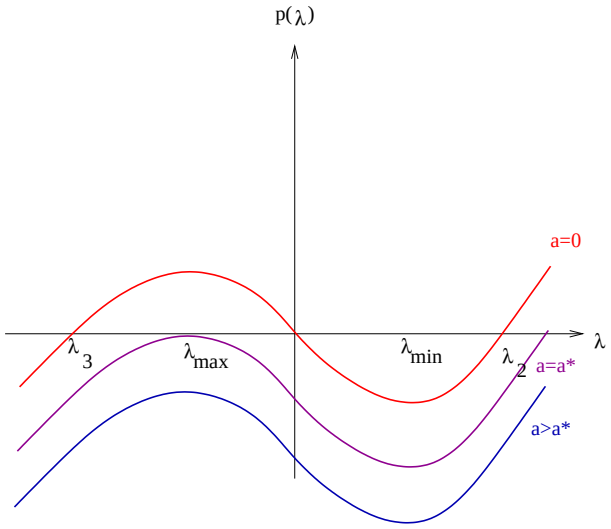
The local maximum and minimum of $p(\lambda)$ are:

$$\lambda_{max}, \lambda_{min} = \frac{1}{3}\left((c - \frac{b}{c}) \pm \sqrt{(c - \frac{b}{c})^2 + 3b}\right)$$

Remark that they are independent of a! For $a = 0$ we can calculate easily the roots of $p(\lambda) = 0$:

$$\lambda_1 = 0, \qquad \lambda_{2,3} = \frac{1}{2}\left((c - \frac{b}{c}) \pm \sqrt{(c - \frac{b}{c})^2 + 4b}\right).$$

The typical graph of $p(\lambda)$ looks as follows:



Remark: Shifting the parameter a obviously just shifts the graph of $p(\lambda)$ up respectively down. Obviously, it depends on the value of a what happens:

- If $0 < a < a^*$: Two negative roots exist
- If $a = a^*$: The two negative roots are equal
- If $a > a^*$: The two negative roots became complex (with negative real parts).

Back to the search of travelling waves:
We could have a connection from $(1, 0, 0)$ to $(b, 1-b, 0)$ and from $(0, 0, 0)$ to $(b, 1-b, 0)$ (remember that $(b, 1-b, 0)$ only has one unstable direction, but two stable directions), i.e. possibly we could find solutions with the boundary conditions

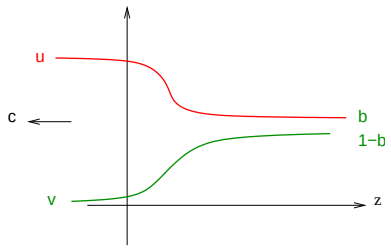
$$U(-\infty) = 1, \quad V(-\infty) = 0, \quad U(\infty) = b, \quad V(\infty) = 1 - b$$

and/or

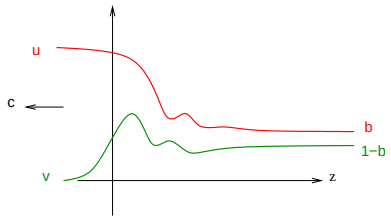
$$U(-\infty)0, \quad V(-\infty) = 0, \quad U(\infty) = b, \quad V(\infty) = 1 - b.$$

From above, we know already that $b < 1$, $c \geq \sqrt{4a(1-b)}$ have to be satisfied. Two different cases may appear:

- For $a < a^*$: monotonic wave profiles, e.g.



- For $a > a^*$: oscillatory wave front solution, e.g.



7.2.3 Travelling fronts in the Belousov-Zhabotinskii Reaction

Reference: [12]

The Belousov-Zhabotinskii reaction is a quite famous chemical reaction system which is able to show up oscillations. Also in the spatial context, it is quite interesting to consider, as it may show up wave phenomena and pattern formation phenomena. Goal: A model for a propagating front of a wave of chemical concentration sin the Belousov-Zhabotinskii reaction!
The (simplified) chemical reaction scheme behind looks as follows:

$$\begin{aligned} A + Y &\xrightarrow{k_1} X + P \\ X + Y &\xrightarrow{k_2} 2P \\ A + X &\xrightarrow{k_3} 2X \\ 2X &\xrightarrow{k_4} P + A, \end{aligned}$$

k_i are the rate constants of the chemical reactions; the product P is not needed for the mathematical analysis. Concentration of A is assumed to be constant. Using the law of mass action and including diffusion for x and y yields as reaction diffusion system:

$$\begin{aligned} \frac{\partial x}{\partial t} &= k_1 a y - k_2 x y + k_3 a x - k_4 x^2 + D \frac{\partial^2 x}{\partial s^2} \\ \frac{\partial y}{\partial t} &= -k_1 a y - k_2 x y + D \frac{\partial^2 y}{\partial s^2} \end{aligned}$$

(remark that s denotes the space variable here). The system can be nondimensionalised,

$$u = \frac{k_4 x}{k_3 a}, \quad v = \frac{k_2 y}{k_3 a r}, \quad s^* = \left(\frac{k_3 a}{D}\right)^{1/2} s, \quad t^* = k_3 a t,$$
$$L = \frac{k_1 k_4}{k_2 k_3}, \quad M = \frac{k_1}{k_3}, \quad b = \frac{k_2}{k_4},$$

and then looks like (removing the asterisks for simplicity)

$$\frac{\partial u}{\partial t} = L r v + u(1 - u - r v) + \frac{\partial^2 u}{\partial s^2} \tag{7.20}$$
$$\frac{\partial v}{\partial t} = -M v - b u v + \frac{\partial^2 v}{\partial s^2} \tag{7.21}$$

When realistic parameters are used, then L and M are of order 10^{-4}, whereas b is of order 1; r is something between 5 and 50 (it has to do something with the given bromide ion concentration).
The (spatially homogeneous) stationary states can be easily computed:

$$(u, v) = (0, 0) \qquad \text{and} \qquad (u, v) = (1, 0).$$

First approximation: Due to $L \ll 1$ and $M \ll 1$, the corresponding terms are neglected, which yields a model for the leading edge of travelling waves in the Belousov-Zhabotinskii reaction:

$$\frac{\partial u}{\partial t} = u(1 - u - r v) + \frac{\partial^2 u}{\partial s^2} \tag{7.22}$$
$$\frac{\partial v}{\partial t} = -b u v + \frac{\partial^2 v}{\partial s^2}. \tag{7.23}$$

Remark: In this approximated model, all states of the form $(0, S)$ ($S > 0$ arbitrary) correspond to stationary solutions.

Search for travelling wavefront solutions of (7.22), (7.23):
Boundary conditions:

$$u(-\infty, t) = 0, \quad v(-\infty, t) = 1, \quad u(\infty, t) = 1, \quad v(\infty, t) = 0,$$

we look for a wave moving to the left.

Short remark in between: If we set

$$v = \frac{1-b}{r}(1-u), \quad b \neq 1, \quad r \neq 0,$$

then the system (7.22), (7.23) obviously reduces to the well-known

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

the Fisher equation. For this case, we know already many details; e.g. the possible travelling speeds ($c \geq 2\sqrt{b}$), for nonnegativity we need $b < 1$; the asymptotic speed dependent on the initial condition was considered, which was (in the notation here) for an initial condition of type

$$u(s, 0) \sim O(exp(-\beta s)) \qquad \text{for } s \to \infty$$

$$c = \begin{cases} \beta + \frac{b}{\beta} & \text{for } 0 < \beta \leq \sqrt{b} \\ 2\sqrt{b}, & \text{for } \beta > \sqrt{b} \end{cases}$$

Of course, assuming $v = \frac{1-b}{r}(1-u)$ is not very realistical; nevertheless, the Fisher equation can be useful for further analysis.
As intial conditions we introduce

$$u(s, 0) = \begin{cases} 0 & \text{for } s < s_1 \\ h(s) & \text{for } s_1 < s < s_2 \\ 1 & \text{for } s_2 < s, \end{cases} \tag{7.24}$$

where $h(s)$ is a positive monotonic continuous function with $h(s_1) = 0$ and $h(s_2) = 1$ (so the desired boundary conditions can be satisfied / smooth transition possible). Then, the solution of the Fisher equation with this initial condition has wave speed $c = 2\sqrt{b}$.
Let $u_f(s, t)$ be the (unique) solution of

$$\frac{\partial u_f}{\partial t} = u_f(1-u_f) + \frac{\partial^2 u_f}{\partial s^2}$$

with boundary conditions

$$u_f(-\infty, t) = 0, \qquad u_f(\infty, t) = 1$$

and initial conditions (7.24); its asymptotic travelling wavefront solution has speed $c = 2$.
Let $u(s, t)$ be a solution of (7.22), (7.23) with the given boundary conditions and initial conditions (7.24). Using the comparison theorem we get

$$u(s, t) \leq u_f(s, t) \qquad \text{for all } s, \quad t > 0.$$

Again, we take the argument that a solution which is bounded above by another function cannot travel faster than the "bound-function", thus there is the upper bound $c(r, b) \leq 2$ for the wave speed of the Belousov-Zhabotinskii solution, for all r, b. One can ask further for the dependency of the wave speed on the parameters b and r. We consider some limiting cases:

- $b = 0$: The v equation becomes $v_t = v_{ss}$, just the diffusion equation, which cannot have a wave solution. As u and v must have the same wave speed, it doesn't work in this case at all, corresponding to $c(b \to 0, r) = 0$ for $r > 0$.
- $b \to \infty$: For v, it follows directly that $v = 0$; excluding the trivial solution $u = 0$ then leads to $c(b \to \infty, r) = 2$ for all $r \geq 0$ (from the standard Fisher equation)

- $r = 0$: Then the u equation is decoupled of v and corresponds to the standard Fisher equation, with wave speed $c = 2$ for the given initial conditions; thus the relevant solution for v also needs to have wave speed 2.
- $r \to \infty$: Either $u = 0$ or $v = 0$, so no wave solution is possible, corresponding to $c(b, r \to \infty) = 0$. (Remark: Here we have a nonuniform limiting situation; the limit $r \to \infty$ with $v \neq 0$ does not correspond to the situation with $v = 0$ and then letting $r \to \infty$, as in the latter case, u is governed by the Fisher equation and r does not play a role).

Of course, we can apply now the classical travelling wave approach, let

$$u(s,t) = f(z), \qquad v(s,t) = g(z) \qquad \text{with } z = s + ct,$$

resulting in

$$\begin{aligned} f'' - cf' + f(1 - f - rg) &= 0 \\ g'' - cg' - bfg &= 0 \end{aligned}$$

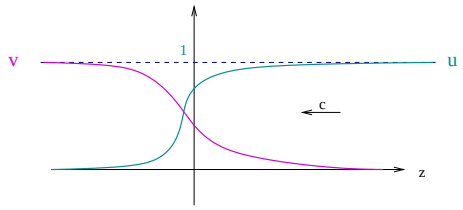
with the boundary conditions

$$f(\infty) = g(-\infty) = 1, \qquad f(-\infty) = g(\infty) = 0.$$

With refined methods (using various bounds and estimation techniques for monotonic, nonnegative solutions), an estimation for c, dependent on the parameters r and b was found by Murray (1976):

$$\left(\left(r^2 + \frac{2b}{3} \right)^{1/2} - r \right) (2(b + 2r))^{-1/2} \leq c \leq 2.$$

Numerically, the typical wavefronts can be computed and look (qualitatively) as follows:



7.2.4 Waves in Excitable Media

Scalar case

Reference: [11]

We consider

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

with

$$f(u) = A(u - u_1)(u_2 - u)(u - u_3).$$

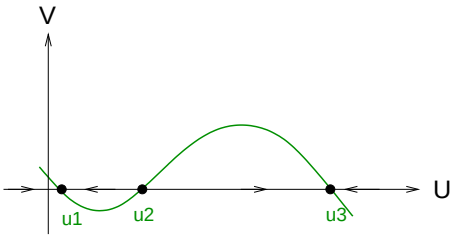
The typical travelling wave approach $u(x,t) = U(z)$ with the wave variable $z = x - ct$ leads to

$$DU'' + cU' + f(U) = 0,$$

which can be transformed into

$$\begin{aligned} U' &= V \\ V' &= -\frac{c}{D}V - \frac{f(U)}{D}. \end{aligned}$$

The system obviously has three stationary points, $(u_1, 0)$, $(u_2, 0)$, $(u_3, 0)$.



For a travelling wave, we look for a connection of $(u_1, 0)$ to $(u_3, 0)$ (for this, the u-value has to exceed u_2 somewhere). So we want to have the boundary conditions

$$U(-\infty) = u_3, \qquad U(\infty) = u_1.$$

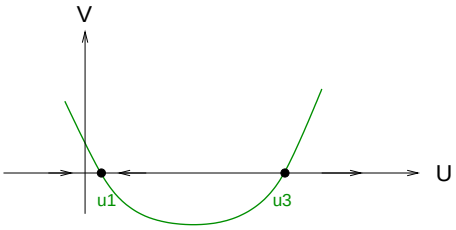
Goal: Determine the wave speed c. Let

$$L(U) = DU'' + cU' + A(U - u_1)(u_2 - U)(U - u_3) = 0. \tag{7.25}$$

Now a trick is used: We do not know yet the explicit form of the solution, but we use another ODE instead of it, which is simpler than (7.25), but behaves somehow similar. The idea is to assume that U satisfies the simpler ODE, but allows to choose parameters, such that it also satisfies (7.25). With this idea behind, let U satisfy

$$U' = a(U - u_1)(U - u_3), \tag{7.26}$$

it also connects u_1 and u_3.



Using

$$\begin{aligned} U'' &= a(U - u_3)U' + a(U - u_1)U' \\ &= a^2(2U - u_1 - u_3)(U - u_1)(U - u_3), \end{aligned}$$

equation (7.26) is taken and substituted into (7.25):

$$\begin{aligned} L(U) &= (U - u_1)(U - u_3)Da^2(2U - u_1 - u_3) + ca(U - u_1)(U - u_3) + A(U - u_1)(u_2 - U)(U - u_3) \\ &= (U - u_1)(U - u_3)\left\{Da^2(2U - u_1 - u_3) + ca + A(u_2 - U)\right\} \\ &= (U - u_1)(U - u_3)\left\{U[2Da^2 - A] - [Da^2(u_1 + u_3) - ca - Au_2]\right\} \end{aligned}$$

The goal was to have $L(U) = 0$, hence we must have

$$2Da^2 - A = 0 \qquad \text{and} \qquad Da^2(u_1 + u_3) - ca - Au_2 = 0,$$

by this, a and c (the wave speed) are uniquely determined:

$$a = \sqrt{A/2D}, \qquad c = Da(u_1 + u_3) + \frac{A}{a}u_2 = \sqrt{AD/2}(u_1 + u_3 - 2u_2).$$

This means: If a and c are chosen in this way, the solutions of (7.26) also can satisfy the "full" equation (7.25).
The solution of (7.26) reads

$$U(z) = \frac{u_3 + Ku_1 \exp(a(u_3 - u_1)z)}{1 + K \exp(a(u_3 - u_1)z)}$$

(the constant K can be chosen arbitrarily), satisfying

$$U(-\infty) = u_3 \qquad \text{and} \qquad U(\infty) = u_1,$$

as desired. Remark that the sign of c may change:
If $u_2 > \frac{u_1+u_3}{2}$, then $c < 0$.
If $u_2 < \frac{u_1+u_3}{2}$, then $c > 0$.

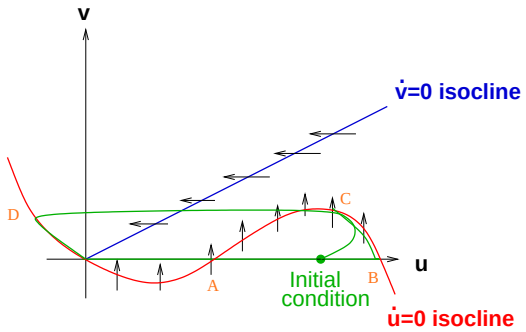
Fitzhugh-Nagumo

Reference: [12]

Here we consider the famous Fitzhugh-Nagumo equations including diffusion.
Short review about these equations, which are somehow a "prototype" for models of excitable media:
The basic reaction equations are formulated as

$$\begin{aligned} \dot{u} &= u(a-u)(u-1) - v \\ \dot{v} &= bu - \gamma v. \end{aligned}$$

They are - somehow - a simplified version of the Hodgkin-Huxley equations, which describe the dynamics of a neuron via a potential (u) and a blocking mechanism (v) (for more details, see e.g. [11]). The nullclines look as follows:



There is just one stationary state, $(0,0)$, which is globally stable, but "excitable". "Excitable" means the following: If a initial condition (respectively a perturbation from the stationary state) which is such that $v = 0$ and $u < a$, then the solution just returns to $(0,0)$. Vice versa, if $u > a$ is chosen / perturbed in that way, then the solution curve takes a larger excursion in u and v before returning to $(0,0)$.
For the potential u diffusion is assumed, leading to the following spatial model:

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + u(a-u)(u-1) - v \tag{7.27}$$

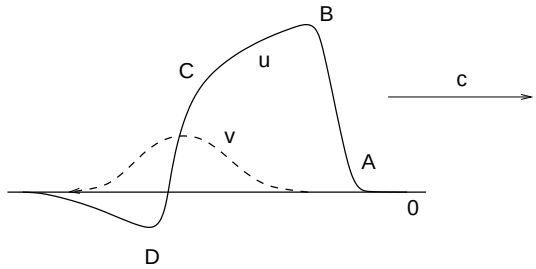
$$\frac{\partial v}{\partial t} = bu - \gamma v. \tag{7.28}$$

Let $f(u) = u(a-u)(u-1)$; we use now the travelling wave coordinate $z = x - ct$, so travelling wave solutions should satisfy

$$Du'' + cu' + f(u) - v = 0 \tag{7.29}$$

$$cv' + bu - \gamma v = 0 \tag{7.30}$$

The important point, if and how a travelling pulse may exist, are the initial conditions - without a perturbation which exceeds the critical value a, the kinetics just brings it back to 0 (i.e. the spatial perturbation "dies out"). A typical travelling pulse looks as follows:



The boundary conditions for a travelling pulse can be formulated as

$$u \to 0, \qquad u' \to 0, \qquad v \to 0 \quad \text{for } |z| \to \infty.$$

The idea now is to consider the different parts of the travelling pulse separately.
As a special case, we consider small b and γ, where

$$b = \varepsilon L, \qquad \gamma = \varepsilon M \qquad \text{for } 0 < \varepsilon \ll 1.$$

Then our system reads

$$\begin{aligned} u_t &= Du_{xx} + f(u) - v \\ v_t &= \varepsilon(Lu - Mv). \end{aligned}$$

If we consider the leading front of the wave pulse $(0AB)$, then for $\varepsilon \to 0$ we have $v \approx const. = 0$, i.e. the system collapses to

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

where $f(u) = u(a-u)(u-1)$. From the scalar excitable system above, we get immediately the wave speed:

$$c = \left(\frac{D}{2}\right)^{1/2}(1-2a).$$

This is only positive, if $a < \frac{1}{2}$.
Next we consider the part BC; obviously there v changes - due to $v_t = O(\varepsilon)$ this takes a long time $(O(\frac{1}{\varepsilon}))$. This can be done by a singular perturbation analysis (left out here).
The next question arises: Where is C positioned on the phase trajectory? For this, it is important to remark that the wave speed of this so-called "trailing edge" has to be the same as for $0AB$, as they have to form one wave pulse. Due to the fast time scale, v doesn't change (much), so we have on this part on the trajectory approximately $v \approx v_C$ and we get the equation

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

For the boundary conditions we need

$$u(-\infty) = u_D, \qquad u(\infty) = u_C.$$

Let u_C, u_D and u_P be the roots of $f(u) = v_C$, then we can use again the scalar example to get an information about the wave speed:

$$c = \sqrt{\frac{D}{2}}(u_C - 2u_P + u_D).$$

If we express u_C, u_D and u_P in terms of v_C, then $c(v_C)$ is a function of v_C. Hence, as the wave speed has to be the same as for $0AB$, c is fixed and by that v_C can be uniquely determined (it is a polynomial which has to be solved).
As a last step, one could consider the part $D0$, called the "refractory phase". This is again a slow process, we leave it out now.

Such threshold waves are also obtained in many other examples, e.g. two-species systems where one of the reactions is fast.

Poincare inequality

Reference: [7]

Often, one considers an ODE of the following form:

$$\frac{d^2y}{dx^2} + \lambda y = 0$$

with the boundary conditions

$$\frac{dy(0)}{dx} = \frac{dy(1)}{dx} = 0.$$

So, we get an "eigenvalue problem" with the eigensolutions

$$\phi_n(x) = \cos n\pi x, \qquad n = 0, 1, 2$$

with $\lambda = \lambda_n = n^2\pi^2$. For any function $w(x)$ which satisfies the boundary conditions and is twice differentiable, the second derivative can be written as

$$\frac{d^2w}{dx^2} = \sum_{n=0}^{\infty} a_n \cos n\pi x \tag{7.31}$$

with the coefficients

$$\begin{aligned} a_0 &= \int_0^1 \frac{d^2w}{dx^2}\,dx = \left[\frac{dw}{dx}\right]_0^1 = 0 \\ a_n &= 2\int_0^1 \frac{d^2w}{dx^2}\cos n\pi x\,dx \qquad \text{for } n \geq 1. \end{aligned}$$

We take (7.31) and integrate it twice, with respect to the boundary condition, thus we get

$$w(x) = \sum_{n=0}^{\infty} -\frac{a_n}{n^2\pi^2}\cos n\pi x + C$$

Remark that

$$\int_0^1 \cos(k\pi x)\cdot\cos(l\pi x)\,dx = \begin{cases} 0 & \text{for } k \neq l \\ \frac{1}{2} & \text{for } k = l \end{cases}$$

Furthermore we find:

$$\begin{aligned} \int_0^1 \left(\frac{dw}{dx}\right)^2 dx &= \underbrace{\left[w\frac{dw}{dx}\right]_0^1}_{=0} - \int_0^1 w\frac{d^2w}{dx^2}\,dx \\ &= \int_0^1 \left(\sum_{n=0}^{\infty}\frac{a_n}{n^2\pi^2}\cos n\pi x\right)\left(\sum_{n=0}^{\infty} a_n\cos n\pi x\right)dx - C\underbrace{\int_0^1 \left(\sum_{n=0}^{\infty} a_n\cos n\pi x\right)dx}_{=0} \\ &= \frac{1}{2}\sum_{n=0}^{\infty}\frac{a_n^2}{n^2\pi^2} \\ &\leq \frac{1}{2\pi^2}\sum_{n=0}^{\infty} a_n^2 \end{aligned} \tag{7.32}$$

and (by taking (7.31), multiplying it by $\frac{d^2w}{dx^2}$ and integrating)

$$\int_0^1 \left(\frac{d^2w}{dx^2}\right)^2 dx = \sum_{n=0}^{\infty} a_n\int_0^1 \frac{d^2w}{dx^2}\cos n\pi x\,dx = \frac{1}{2}\sum_{n=0}^{\infty} a_n^2$$

(this is the Parseval equality!)
We insert this Parseval equality into (7.32) and get

$$\int_0^1 \left(\frac{dw}{dx}\right)^2 dx \leq \frac{1}{\pi^2}\int_0^1 \left(\frac{d^2w}{dx^2}\right)dx, \tag{7.33}$$

which is called the "Poincare inequality".

Criteria for a pulse

Reference: [7]

We can consider in greater detail the conditions how the threshold has to be exceeded to cause really a peak, or - vice versa - which conditions still just lead to a decay effect. For that purpose we consider the Fitzhugh-Nagumo equations (7.27), (7.28) with the following conditions for a stimulus at $x = 0$ which act over a finite time interval:

$$u(0,t) = P(t) \qquad u(x,0) = 0 \tag{7.34}$$

$$v(0,t) = b\int_0^t P(s)e^{-\gamma s}ds \qquad v(x,0) = 0 \tag{7.35}$$

and, as the stimulus only should at during a finite time interval, $P(t) = 0$ for $t \geq T$.
Further assumptions: $u(x,t)$, $v(x,t)$ tend to 0 for $x \to \infty$, such that $\int_0^\infty u^2(x,t)\,dx$, $\int_0^\infty v^2(x,t)\,dx$ exist

and are finite for all t. For simplicity, we assume $D = 1$ in the following.
Next, (7.27) is multiplied by bu and (7.28) is multiplied by v; subtracting the resulting equations yields

$$\begin{aligned} bu\frac{\partial^2 u}{\partial x^2} - v\frac{\partial v}{\partial t} &= bu\frac{\partial u}{\partial t} - bu^2(1-u)(u-a) + buv - buv - \gamma v^2 \\ \Leftrightarrow \quad bu\frac{\partial u}{\partial t} + v\frac{\partial v}{\partial t} &= bu\frac{\partial^2 u}{\partial x^2} + bu^2(1-u)(u-a) - \gamma v^2 \\ \Leftrightarrow \quad \frac{1}{2}\frac{\partial}{\partial t}(bu^2+v^2) &= b\frac{\partial}{\partial x}(u\frac{\partial u}{\partial x}) - b(\frac{\partial u}{\partial x})^2 + bu^2(1-u)(u-a) - \gamma v^2 \end{aligned}$$

This equation is integrated over x (apply the initial condition (7.34), then it follows for $t \geq T$:

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\int_0^\infty (bu^2+v^2)\,dx &= \underbrace{\int_0^\infty b\frac{\partial}{\partial x}(u\frac{\partial u}{\partial x})\,dx}_{=0} - b\int_0^\infty (\frac{\partial u}{\partial x}^2\,dx + \int_0^\infty (bu^2(1-u)(u-a) - \gamma v^2)\,dv \\ &\leq \int_0^\infty (bu^2(1-u)(u-a) - \gamma v^2)\,dx \end{aligned}$$

Let $u(x,t) < a$ for all x, $t > 0$, then the following estimate can be used for a constant δ (δ depends on a):

$$u^2(1-u)(u-a) \leq -\delta u^2.$$

If we use this above, we get

$$\frac{1}{2}\frac{d}{dt}\int_0^\infty (bu^2+v^2)\,dx \leq -\int_0^\infty (b\delta u^2 + \gamma v^2)\,dx.$$

Let $C = \min\{\delta, \gamma\}$, then it can be rewritten as

$$\frac{d}{dt}\int_0^\infty (bu^2+v^2)\,dx \leq -2C\int_0^\infty (bu^2+v^2)\,dx,$$

which yields in the end the estimate

$$\int_0^\infty (bu^2+v^2)\,dx \leq Ke^{-2Ct}.$$

The result is: Starting with an action potential below the potential value a leads to an exponential decay in time for the mean square of $u(x,t)$. One can show a more precise statement (without proof here): Let $a > \frac{b}{\gamma}$ and $P(t)$ bounded, continuous and satisfying the conditions

(i) $P(t) = P(0) = 0$ for all $t \geq T > 0$

(ii) $\sup_{t\geq 0} |P(t)| \leq M$.

Then

$$\sup_{x\geq 0} |u(x,t)| \leq k\int_0^t |P(s)|\,ds \qquad \text{for all } t \geq T$$

and there are constants C, k, λ such that if $\int_0^T |P|\,dt < \lambda$, then

$$\sup_{x\geq 0} |u(x,t)| \leq k\exp(-Ct), \qquad t \geq 0.$$

Also possible to show: If M is sufficiently small, then

$$\sup_{x\geq 0} |u(x,t)| \leq k\exp(-Ct), \qquad t \geq 0.$$

Now we consider a more realistic problem with finitely long nerves (length l). At $x = 0$ we start again with

$$\begin{aligned} u(0,t) &= P(t) \\ v(0,t) &= b\int_0^t P(s)e^{-\gamma s}\,ds. \end{aligned}$$

At $x = l$, one could assume either a Dirichlet condition

$$u(l,t) = 0 \qquad \text{for } t \geq 0$$

or Robin condition

$$\frac{\partial u(l,t)}{dx} - \alpha u(l,t) = 0, \qquad \text{for } t \geq 0, \alpha \leq 0$$

For $P(t)$ we assume that $P(t) = 0$ for $t \geq T$.
(7.27) is multiplied by u, (7.28) is multiplied by $b^{-1}v$, subtracting yields

$$\frac{1}{2}\frac{\partial}{\partial t}(u^2 + \frac{v^2}{b}) = u\frac{\partial^2 u}{\partial x^2} + u^2(1-u)(u-a) - \frac{\gamma}{b}v^2,$$

integrating yields

$$\frac{1}{2}\int_0^l \frac{\partial}{\partial t}(u^2 + \frac{v^2}{b})\,dx = \int_0^l (u\frac{\partial^2 u}{\partial x^2} + u^2(1-u)(u-a) - \frac{\gamma}{b}v^2)\,dx.$$

Remark that

$$\int_0^l u\frac{\partial^2 u}{\partial x^2}\,dx = \left[u\frac{\partial u}{\partial x}\right]_0^l - \int_0^l \left(\frac{\partial u}{\partial x}\right)^2 dx,$$

taking into account the boundary condition $u(0,t) = 0 = u(l,t)$, $t \geq T$, results in

$$\int_0^l u\frac{\partial^2 u}{\partial x^2}\,dx = -\int_0^l \left(\frac{\partial u}{\partial x}\right)^2 dx.$$

Analogously, for the Robin condition $u(0,t) = 0 = \frac{\partial}{\partial x}u(l,t) - \alpha u(l,t)$, $t \geq T$, we find

$$\int_0^l u\frac{\partial^2 u}{\partial x^2}\,dx = \underbrace{\left[u\frac{\partial u}{\partial x}\right]_0^l}_{=\alpha u^2(l,t)} - \int_0^l (\frac{\partial u}{\partial x})^2\,dx \leq -\int_0^l (\frac{\partial u}{\partial x})^2\,dx$$

due to $\alpha \leq 0$.
For both cases we get

$$\frac{1}{2}\frac{\partial}{\partial t}\int_0^l (u^2 + \frac{v^2}{b})\,dx \leq \int_0^l (u^2(1-u)(u-a) - \frac{\gamma}{b}v^2)\,dx - \int_0^l (\frac{\partial u}{\partial x})^2\,dx.$$

Remark that the term $(1-u)(u-1)$ has a maximum at $u = \frac{(1-a)}{2}$ and assumes there the value $\frac{(1-a)^2}{4}$, so we can use this estimate and get

$$\frac{1}{2}\frac{\partial}{\partial t}\int_0^l (u^2 + \frac{v^2}{b})\,dx \leq \int_0^l \left(\frac{(1-a)^2}{4}u^2 - \frac{\gamma}{b}v^2 - (\frac{\partial u}{\partial x})^2\right) dx.$$

For the Dirichlet boundary conditions $u(0,t) = 0 = u(l,t)$, $t \geq T$, we can directly apply the Poincare inequality (7.33), which reads in our case

$$\int_0^l (\frac{\partial u}{\partial x})^2\,dx \geq (\frac{\pi}{l})^2 \int_0^l u^2\,dx$$

Remark that the conditions for the Poincare inequality are satisfied by using $u = \frac{dw}{dt}$. This also works in a similar way for the Robin boundary condition at $x = l$.
So we get

$$\frac{1}{2}\frac{\partial}{\partial t}\int_0^l (u^2 + \frac{v^2}{b})\,dx \leq \int_0^l \left((\frac{(1-a)^2}{4} - \frac{\pi^2}{l^2})u^2 - \frac{\gamma}{b}v^2\right) dx.$$

Considering that case with $l < \frac{2\pi}{(1-a)} \Leftrightarrow \frac{(1-a)^2}{4} - \frac{\pi^2}{l^2} < 0$, one can formulate

$$\frac{\partial}{\partial t}\int_0^l (u^2 + \frac{v^2}{b})\,dx \leq -2C\int_0^l (u^2 + \frac{v^2}{b})\,dx,$$

where C is chosen as

$$C = \max\left\{\frac{\pi^2}{l^2} - \frac{(1-a)^2}{4}, \gamma\right\}.$$

Using this formulation, it follows again, that

$$\int_0^l (u^2 + \frac{v^2}{b})\, dx$$

decays exponentially.
What does this mean from a biological point of view? If l (the length of the axon) is not sufficiently long, then all stimuli decay exponentially in time. Nevertheless, also an infinitely long axon may not propagate a stimulus, but it is not completely clear until now, how $P(t)$ really has to look like, such that a propagation of an action potential is possible.

For some more details concerning the influence of the axon length on the behaviour of possible solutions, see e.g. [2]

7.2.5 Travelling Wave Trains in Reaction Diffusion Systems with Oscillatory Kinetics

Reference: [12]

In this subsection, we consider reaction diffusion systems with reaction terms that possess limit cycles; one can expect wavetrain solutions when including diffusion. In general such systems look like

$$\frac{\partial u}{\partial t} = f(u) + \frac{\partial^2 u}{\partial x^2} \tag{7.36}$$

For the reaction term, i.e. the spatially homogeneous system, we assume a dependency on a parameter (which is used as bifurcation parameter later), so

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

For $\gamma < \gamma_c$ it is assumed to possess a stable stationary state, and a Hopf bifurcation appears at $\gamma = \gamma_c$, such that the stationary state looses its stability and a stable limit cycle solutions appears (at least for $\gamma = \gamma_c + \varepsilon$ where $0 < \varepsilon \ll 1$).
Now we look for a travelling plane wavetrain solution, thus we use the approach

$$u(x,t) = U(z), \qquad z = \sigma t - kx,$$

where U is a 2π-periodic function of z, the so-called "phase". (Remark that this is just a slight generalisation of the former approach, using the frequency $\sigma > 0$ and the wavenumber k; resulting in the wavelength $\omega = 2\pi/k$ and the wavespeed $c = \sigma/k$). We insert this approach into (7.36): and get the following ODE system:

$$k^2 U'' - \sigma U' + f(U) = 0$$

How to choose σ and k such that this equation has a 2π periodic solution U?
As a special case, we consider the so-called $\lambda - \omega$ system as a prototype for such a system. It includes two reactants u and v and reads

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \lambda(r) & -\omega(r) \\ \omega(r) & \lambda(r) \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} + \frac{\partial^2}{\partial x^2}\begin{pmatrix} u \\ v \end{pmatrix}, \tag{7.37}$$

where $r^2 = u^2 + v^2$; $\lambda(r)$ and $\omega(r)$ are real functions of r. For guaranteeing the limit cycle solution, we need an isolated zero $r_0 > 0$ of $\lambda(r)$, $\lambda'(r_0) < 0$ and $\omega(r_0) \neq 0$.
Next we change the used variables (u, v) into polar coordinates (r, θ), via

$$u = r\cos\theta, \qquad v = r\sin\theta. \tag{7.38}$$

The transformed system becomes

$$r_t = r\lambda(r) + r_{xx} - r\theta_x^2 \tag{7.39}$$

$$\theta_t = \omega(r) + \frac{1}{r^2}(r^2\theta_x)_x. \tag{7.40}$$

If the isolated zero $r_0 > 0$ of $\lambda(r)$ exists and the condition $\lambda'(r_0)$ is also satisfied, then we can see immediately the limit cycle solution of the kinetics:

$$r = r_0 \qquad \text{and} \qquad \theta = \theta_0 + \omega(r_0)t.$$

(θ_0 is an arbitrary phase). Retransforming this result via (7.38) yields the limit cycle solution in the original variables u and v:

$$u = r_0 \cos(\omega(r_0)t + \theta_0), \qquad v = r_0 \sin(\omega(r_0)t + \theta_0),$$

they also have frequency $\omega(r_0)$ and amplitude r_0.

If we now look for a travelling plane wave solution as introduced above, i.e. $u(x,t) = U(z)$, $v(x,t) = V(t)$ and $z = \sigma t - kx$, then they read in the polar form

$$r = \alpha, \qquad \theta = \sigma t - kx,$$

due to the claim that U, V are periodic (sin, cos with period 2π (thus the radius has to be constant and θ shows the desired behaviour). (Remark: Then $u = r\cos\theta$ and $v = r\sin\theta$ are periodic as desired)
Inserting this approach into (7.39) yields

$$\begin{aligned} 0 &= \alpha\lambda(\alpha) - \alpha k^2 \\ \sigma &= \omega(\alpha) + \frac{1}{\alpha^2}(\alpha^2(-k))_x, \end{aligned}$$

thus

$$\sigma = \omega(\alpha) \qquad \text{and} \qquad k^2 = \lambda(\alpha). \tag{7.41}$$

Using α as the "relevant" parameter yields a one-parameter family of travelling wave train solutions of the two-reactants model which can be written as

$$\begin{aligned} u &= \alpha\cos(\omega(\alpha t - x\lambda^{1/2}(\alpha)) \\ v &= \alpha\sin(\omega(\alpha)t - x\lambda^{1/2}(\alpha)). \end{aligned}$$

The corresponding wave speed is

$$c = \frac{\sigma}{k} = \frac{\omega(\alpha)}{\lambda^{1/2}(\alpha)}.$$

Letting $r = \alpha$ tend to r_0 with the conditions from above, this means that there is the limit cycle solution, where $\lambda(r) \to 0$ by definition; correspondingly $k \to 0$ (k was the wave number).

We consider an example:

$$\omega(r) = 1, \qquad \lambda(r) = \gamma - r^2$$

The reaction dynamics,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \lambda(r)u - \omega(r)v = (\gamma - (u^2+v^2))u - v \\ \frac{\partial v}{\partial t} &= \omega(r)u + \lambda(r)v = u + (\gamma - (u^2+v^2))v, \end{aligned}$$

has a stationary point at $(u,v) = (0,0)$.
The Jacobian matrix reads

$$\begin{pmatrix} \gamma - 3u^2 - v^2 & -1 \\ 1 & \gamma - u^2 - 3v^2 \end{pmatrix},$$

i.e. in $(0,0)$: $\begin{pmatrix} \gamma & -1 \\ 1 & \gamma \end{pmatrix}$, the characteristic polynomial reads $(\gamma - \lambda)^2 + 1 = 0$, thus

$$\lambda^2 - 2\gamma\lambda + \gamma^2 + 1 = 0 \qquad \Leftrightarrow \qquad \lambda_{1,2} = \frac{2\gamma \pm \sqrt{4\gamma^2 - 4(\gamma^2+1)}}{2} = \gamma \pm i.$$

Hence, obviously $(0,0)$ is stable for $\gamma < 0$ and unstable for $\gamma > 0$. Using γ as bifurcation parameter for $\gamma_c = 0$, the eigenvalues are $\pm i$, satisfying the standard Hopf bifurcation requirement. Thus, for $\gamma = \gamma_c + \varepsilon$

with $0 < \varepsilon \ll 1$ limit cycle solutions with small amplitude can be expected. For $r = \sqrt{\gamma}$ we get $\lambda = 0$ and from above we know that the limit cycle solutions are given by

$$\begin{aligned} u_\gamma(t) &= \sqrt{\gamma}\cos t \\ v_\gamma(t) &= \sqrt{\gamma}\sin t, \qquad \text{where } \gamma > 0, \end{aligned}$$

or, written in polar variables

$$r_0 = \sqrt{\gamma}, \qquad \theta = t + \theta_0$$

(the arbitrary phase θ_0 can be chosen to be 0).
Next, we consider the complete system with diffusion, i.e.

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \gamma - r^2 & -1 \\ 1 & \gamma - r^2 \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} + \frac{\partial^2}{\partial x^2}\begin{pmatrix} u \\ v \end{pmatrix},$$

we look for travelling wave solutions of the form

$$r = r_0, \qquad \theta = \sigma t - kx$$

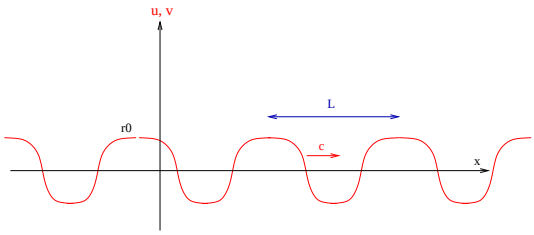
and get from (7.41) immediately

$$\sigma = 1, \qquad k^2 = \gamma - r_0^2,$$

thus $0 < r_0 < \sqrt{\gamma}$.
The corresponding small amplitude wavetrain solutions are

$$\begin{aligned} u &= r_0\cos(t - x\sqrt{\gamma - r_0^2}) \\ v &= r_0\sin(t - x\sqrt{\gamma - r_0^2}). \end{aligned}$$

They look as follows:



The amplitude satisfies $r_0 < \sqrt{\gamma}$, the wavelength is $L = \frac{2\pi}{k} = \frac{2\pi}{\sqrt{\gamma - r_0^2}}$. The wave speed is $c = \frac{\sigma}{k} = (\gamma - r_0^2)^{-1/2}$

These travelling wavetrains are only of practical relevance, if they are stable. This is quite complicated to show in general.

So, if the reaction kinetics itself shows up periodic behaviour, then adding diffusion is expected to generate travelling periodic wavetrain solutions. In our example of the λ-ω system with the nonlinearity $\lambda(r) = \gamma - r^2$ it was a typical phenomenon of a Hopf bifurcation problem. Next we consider a more general reaction diffusion system with the same property and see that it is similar to λ-ω systems near the Hopf bifurcation.
We consider the following more general two-species system

$$u_t = D\Delta u + F(u, v; \gamma) \tag{7.42}$$
$$v_t = D\Delta v + G(u, v; \gamma) \tag{7.43}$$

F and G are the reaction terms; we assume (just for simplicity) that the system (7.42), (7.43) has a stationary state at $u = v = 0$ and the system without diffusion shows a Hopf bifurcation at the bifurcation value $\gamma = \gamma_c$.
In the next step we consider u and v as perturbations around $(0, 0)$ and use a new notation:

$$T = \begin{pmatrix} u \\ v \end{pmatrix}, \qquad M = \begin{pmatrix} F_u & F_v \\ G_u & G_v \end{pmatrix}_{u=v=0}, \qquad P = \begin{pmatrix} D & 0 \\ 0 & D \end{pmatrix}.$$

Using this notation we can write the full system as

$$T_t = MT + P\Delta T + H, \qquad \text{where } H = \begin{pmatrix} f(u,v;\gamma) \\ g(u,v;\gamma) \end{pmatrix},$$

then f and g denote the nonlinear contribution of F and G to u and v near $u = v = 0$; or the linearised form is

$$T_t = MT + P\Delta T.$$

According to the assumption, the kinetics has a Hopf bifurcation at $\gamma = \gamma_c$. This means, in the new notation, that the eigenvalues of the matrix M (denoted by σ) have the property that

$$Re\sigma(\gamma) < 0 \text{ for } \gamma < \gamma_c$$

$$Re\sigma(\gamma_c) = 0, \qquad Im\sigma(\gamma_c) \neq 0$$

$$Re\sigma(\gamma) > 0 \text{ for } \gamma > \gamma_c.$$

This means: at $\gamma = \gamma_c$ we have

$$trM = 0, \qquad detM > 0, \qquad \text{thus } \sigma(\gamma_c) = \pm i(detM)^{1/2}.$$

We introduce a constant matrix N and a nonconstant matrix W which satisfy

$$T = NW.$$

Then it follows:

$$W_t = N^{-1}MNW + N^{-1}PN\Delta W + N^{-1}H \tag{7.44}$$

(using the full system equation). We choose N in such a way that

$$N^{-1}MN = \begin{pmatrix} 0 & -k \\ k & 0 \end{pmatrix}$$

at $\gamma = \gamma_c$, hence we get $k^2 = detM|_{\gamma=\gamma_c}$. So, in the linearised system we have the coefficients in the linearised matrix:

$$N^{-1}MN = \begin{pmatrix} \alpha(\gamma) & -\beta(\gamma) \\ \beta(\gamma) & \delta(\gamma) \end{pmatrix},$$

where

$$\alpha(\gamma_c) = 0 = \delta(\gamma_c), \quad \beta(\gamma_c) \neq 0.$$

Remark: This corresponds to the λ-ω form near the bifurcation γ_c. Hence we have found: The general system (7.42), (7.43) with a Hopf bifurcation at the stationary state can be transformed into a system in λ-ω form near γ_c. So many results for λ-ω systems can be carried over to other reaction diffusion system (which are e.g. more realistic).

One can show the same thing for different diffusion coefficients.

7.3 Spiral waves

Reference: [7, 12]

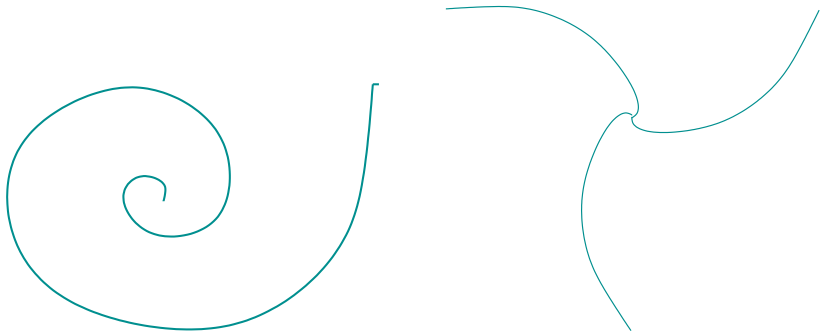
There are many applications which show up spiral waves, e.g. quite famous is the Belousov Zhabotinskii system exhibits spiral waves in 2D (or also in 3D, as "scroll waves"). But there are also other examples like the electrochemical waves through the cortex (brain tissue), or in the signalling pattern of the slime mould *Dictyostelium discoideum*. This means, there are time-periodic, rotating spatial structures of the considered densities / concentrations / potentials. If one considers such a situation at a fixed time point, one can see a typical spiral pattern; in time course the whole spiral pattern is rotating. Remark that the wavefronts correspond to isoconcentrations lines.
What does it mean from a mathematical point of view? We consider a spiral wave which rotates around its centre. Choosing a fixed position in space, somehow a periodic wavetrain passes there. Let ϕ describe the concentration of a reactant, which is described by its phase. A simple spiral wave can be written as a periodic function of ϕ (using polar coordinates r and θ), and ϕ is defined by

$$\phi = \Omega t \pm m\theta + \psi(r). \tag{7.45}$$

Ω denotes the frequency, m the number of arms in the spiral and $\psi(r)$ describes the type of the spiral. Remark that $\pm$ (in the $m\theta$ term) marks the sense of rotation.
E.g. if $\phi = 0$ is set, and the steady state is considered, one gets a description of the spiral forms by specifying the function $\psi(r)$. Typical examples are:

(a) $m = 1$ (i.e. one arm) and $\psi(r) = ar$ (with $a > 0$), the so-called Archimedian spiral

(b) $m = 3$ (i.e. three arms) and $\psi(r) = a \ln r$ (with $a > 0$), the so-called logarithmic spiral



Correspondingly, spirals about a central core at r_0 can be described e.g. by $\theta = a(r - r_0)$ respectively $\theta = a \ln(r - r_0)$.
Altogether, such a spiral configuration (denoted by u) can be described mathematically by

$$u(r, \theta, t) = F(\phi);$$

here $F(\phi)$ is a 2π -periodic function of phase ϕ, which was introduced in (7.45).
Again, for a fixed time t, one can see a "snapshot" of the spiral. By fixing r and t, one gets a circle around the centre with m-fold symmetry (m was the number of arms). Fixing r and θ (i.e. a fixed point in space) allows to consider the passing wavefronts. Obviously, if a wavefront passes at time $t = t_0$ and $\phi = \phi_0$, then the next wavefront will pass at time $t = t_0 + 2\pi/\Omega$ (and $\phi = \phi_0 + 2\pi$).
In some sense, there is a wavelength associated with the spiral (imagine a snapshot), which may vary if we move out from the centre. E.g. if one wavefront is at r_1 and the next one at r_2 (when moving out straightforward), then the wavelength λ can be defined by

$$\lambda = r_2 - r_1, \qquad \theta(r_2) = \theta(r_1) + 2\pi.$$

Now we take (7.45) and fix t, then along the curve $\phi = constant$ it holds

$$\phi_\theta + \phi_r \left[\frac{dr}{d\theta}\right]_{\phi=constant} = 0,$$

which can be reformulated by using the concrete term $-m\theta$ in (7.45) to

$$\left[\frac{dr}{d\theta}\right]_{\phi=constant} = -\frac{\phi_\theta}{\phi_r} = \frac{m}{\psi'(r)},$$

which is called the "pitch" of the spiral - and kind of measure between two wavefronts.
Examples:

- Archimedian spiral: $\psi'(r) = a \rightsquigarrow \left[\frac{dr}{d\theta}\right]_{\phi=constant} = \frac{m}{a}$, i.e. a constant pitch
- Logarithmic spiral: $\psi'(r) = \frac{1}{r} \rightsquigarrow \left[\frac{dr}{d\theta}\right]_{\phi=constant} = \frac{mr}{a}$, i.e. for large r the pitch becomes large and loosely wound, but for small r, the spiral is quite tightly wound.

The wavelength $\lambda(r)$ can then be computed by

$$\lambda(r) = \int_{\theta(r)}^{\theta(r)+2\pi} \left[\frac{dr}{d\theta}\right] d\theta = \int_{\theta(r)}^{\theta(r)+2\pi} \left[\frac{m}{\psi'(r(\theta))}\right] d\theta$$

Remark that r is used here as function of θ, it is given by (7.45) for $t = const.$ and $\phi = const$ (one can choose them to be 0), 1-armed spiral.

As it is quite complicated to look for spiral wave solutions in general reaction diffusion systems and to analyse them, we consider here exemplarily the $\lambda - \omega$ system (which we know already a little bit, see (7.37)). It exhibits the main features and is still accessible by some analysis.

$$\frac{\partial}{\partial t}\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} \lambda(a) & -\omega(a) \\ \omega(a) & \lambda(a) \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} + D\Delta\begin{pmatrix} u \\ v \end{pmatrix}, \tag{7.46}$$

using here $a^2 = u^2 + v^2$. u and v describe the reactant concentrations, $\omega(a)$ and $\lambda(a)$ are real functions of a, and Δ denotes here the 2D Laplacian operator, i.e.

$$\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

One important requirement is that in case of $D = 0$ (no diffusion) the remaining ODE system has a stable limit cycle. For that, $\lambda(a)$ needs an isolated zero (at $a = a_0 > 0$) with $\frac{d\lambda}{da} < 0$ at $a = 0$ and $\omega(a_0) \neq a_0$. Then, the limit cycle is $u^2 + v^2 = a_0$ with the cycle frequency $\omega(a_0)$.
In the next step, we introduce the complex variable $w = u + iv$. The advantage is that we can write the λ-ω system (7.46) in a single complex equation:

$$\frac{\partial w}{\partial t} = (\lambda + i\omega)w + D\Delta w. \tag{7.47}$$

For this system, we look for a solution of the form

$$w = A\exp(i\phi).$$

In this notation, A denotes the amplitude and ϕ the phase of the solution. As usual, this approach is inserted into (7.47) and we get:

$$\begin{aligned} \frac{\partial A}{\partial t}\exp(i\phi) + iA\exp(i\phi)\frac{\partial \phi}{\partial t} &= (\lambda + i\omega)A\exp(i\phi) + D\nabla\cdot(\nabla A\cdot\exp(i\phi) + iA\exp(i\phi)\cdot\nabla\phi) \\ &= (\lambda + i\omega)A\exp(i\phi) + D\Delta A\cdot\exp(i\phi) + D\nabla A\cdot i\exp(i\phi)\nabla\phi \\ &\quad + iD\nabla A\cdot\exp(i\phi)\nabla\phi + DAi^2\nabla\phi\cdot\nabla\phi\cdot\exp(i\phi) + DAi\Delta\phi\exp(i\phi) \end{aligned}$$

The term $\exp(i\phi)$ can be cancelled out and we separate real and imaginary part:

$$\begin{aligned} \frac{\partial A}{\partial t} &= \lambda(a)A + D\Delta A - DA|\nabla\phi|^2 \\ A\frac{\partial \phi}{\partial t} &= \omega(a)A + 2D(\nabla A\cdot\nabla\phi) + DA\Delta\phi \\ \Leftrightarrow\quad \frac{\partial \phi}{\partial t} &= \omega(a) + 2\frac{D}{A}(\nabla A\cdot\nabla\phi) + D\Delta\phi. \end{aligned}$$

Again we use polar coordinates as an appropriate coordinate system for spiral waves, i.e. we look for solutions of the form

$$A = A(r), \qquad \phi = \Omega t + m\theta + \psi(r).$$

Auxiliary reformulations (for the polar coordinates):

$$\begin{aligned} \Delta A &= \frac{\partial^2 A}{\partial r^2} + \frac{1}{r}\frac{\partial A}{\partial r} + \underbrace{\frac{1}{r^2}\frac{\partial^2 A}{\partial \theta^2}} = 0 \text{ in our example} \\ \Delta\phi &= \frac{\partial^2\phi}{\partial r^2} + \frac{1}{r}\frac{\partial\phi}{\partial r} + \frac{1}{r^2}\frac{\partial^2\phi}{\partial\theta^2} = \frac{d^2\psi}{dr^2} + \frac{1}{r}\frac{d\psi}{dr} \qquad \text{(in the example)} \\ \nabla &= \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{1}{r}\frac{\partial}{\partial\theta} \end{pmatrix} \\ \nabla A &= \begin{pmatrix} \frac{\partial A}{\partial r} \\ 0 \end{pmatrix} \\ \nabla\phi &= \begin{pmatrix} \frac{\partial\phi}{\partial r} = \frac{d\psi}{dr} \\ \frac{1}{r}m \end{pmatrix}. \end{aligned}$$

(remark that $\frac{\partial A}{\partial t} = 0$ and $\frac{\partial \phi}{\partial t} = \Omega$) .
Using this approach and the polar coordinates we get as the two equations

$$\begin{aligned} 0 &= \lambda(a)A + D\left(\frac{\partial^2 A}{\partial r^2} + \frac{1}{r}\frac{\partial A}{\partial r}\right) - DA\left((\frac{d\psi}{dr})^2 + \frac{m^2}{r^2}\right) \\ \Omega &= \omega(a) + 2\frac{D}{A}\left(\frac{\partial A}{\partial r}\cdot\frac{d\psi}{dr}\right) + D\left(\frac{d^2\psi}{dr^2} + \frac{1}{r}\frac{d\psi}{dr}\right) \end{aligned}$$

which can be rearranged to

$$D\frac{d^2A}{dr^2} + \frac{D}{r}\frac{dA}{dr} + \left(\lambda(a) - D(\frac{d\psi}{dr})^2 - \frac{Dm^2}{r^2}\right)A = 0 \tag{7.48}$$

$$D\frac{d^2\psi}{dr^2} + D\left(\frac{1}{r} + \frac{"}{A}\frac{dA}{dr}\right)\frac{d\psi}{dr} = \Omega - \omega(a) \tag{7.49}$$

Equation (7.49) can be multiplied by rA^2,

$$\underbrace{DrA^2\frac{d^2\psi}{dr^2} + D(A^2 + 2rA\frac{dA}{dr})\frac{d\psi}{dr}}_{\frac{d}{dr}(DrA^2\frac{d\psi}{dr})} = rA^2(\Omega - \omega(a))$$

and integrated, this yields (have in mind that a corresponds to A)

$$\frac{d\psi}{dr} = \frac{1}{DrA^2(r)}\int_0^r sA^2(s)(\Omega - \omega(A(s)))\,ds$$

Next, we need BCs. Two main properties are required: The solutions have to be regular at $r = 0$ and bounded for $r \to \infty$. For the regularity in (7.48) we have to get rid of the term $-Dm^2/r^2$ and with this result, the term with $2/A$ have to be brought to 0, thus

$$A(0) = 0, \qquad \frac{d\psi}{dr}(0) = 0.$$

Assume that $A \to A_\infty$ for $r \to \infty$. From (7.49) we can use the asymptotic approximation

$$\frac{d\psi}{dr} \sim \frac{1}{DrA_\infty^2}\int_0^r sA_\infty^2(\Omega - \omega(A_\infty))\,ds = \frac{(\Omega - \omega(A_\infty))r}{2D}.$$

Obviously, $\frac{d\psi}{dr}$ is bounded if and only if $\Omega = \omega(A_\infty)$; i.e. the amplitude of the spiral at infinity determines the frequency).
Letting $r \to \infty$ in (7.48) it is

$$\lambda(A_\infty) - D\left(\frac{d\psi(\infty)}{dr}\right)^2 = 0 \qquad \Leftrightarrow \qquad \frac{d\psi(\infty)}{dr} = \left(\frac{\lambda(A_\infty)}{D}\right)^{1/2}.$$

For considering the structure of the spiral near $r = 0$ we use a series of the following form:

$$A(r) = r^c\sum_{n=0}^{\infty} a_n r^n, \qquad a_0 \neq 0.$$

Auxiliary computations:

$$\begin{aligned} \frac{dA(r)}{dr} &= cr^{c-1}\sum_{n=0}^{\infty} a_n r^n + r^c \underbrace{\sum_{n=1}^{\infty} a_n n r^{n-1}}_{\sum_{n=0}^{\infty} a_{n+1}(n+1)r^n} \\ \frac{d^2A(r)}{dr^2} &= c(c-1)r^{c-2}\sum_{n=0}^{\infty} a_n r^n + 2cr^{c-1}\underbrace{\sum_{n=1}^{\infty} a_n n r^{n-1}}_{\sum_{n=0}^{\infty} a_{n+1}(n+1)r^n} \\ &\quad + \underbrace{r^c\sum_{n=1}^{\infty} a_{n+1}(n+1)nr^{n-1}}_{\sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)r^n} \end{aligned}$$

This is inserted into (7.48), compare the terms of the same power in r on both sides; for the lowest order (which is here r^{c-2}) we find

$$D(c(c-1)a_0) + dCa_0 - Dm^2 a_0 = 0 \qquad \Leftrightarrow c(c-1) + c - m^2 = 0 \qquad \Leftrightarrow c^2 - m^2 = 0,$$

this condition has to be satisfied. We still want A to be regular at $r = 0$, thus we need $c = m$. Hence we find (using $w = A\exp(i\phi)$ and the spiral approach) for the structure of u and v near $r = 0$:

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} r^m \cos(\Omega t + m\theta + \psi(0)) \\ r^m \sin(\Omega t + m\theta + \psi(0)) \end{pmatrix}$$

Remark that this is only a quite rough approximation. The correct analytic solutions of such systems are quite difficult or even impossible to obtain; but of course it is possible to examine the structure by numerical approaches. (Sometimes, one also uses such an approximate analysis for $r \to \infty$).

Examples (taken from [12])):
One example for a $\lambda - \omega$ system is

$$\lambda(a) = 1 - A^2, \qquad \omega(a) = -\beta A^2$$

(a and A correspond to each other) with $\beta > 0$. E.g. 1-armed and 2-armed spirals can be computed $\rightsquigarrow$ see Fig. 1.22 in [12]
Another example for a $\lambda - \omega$ system:

$$\lambda(a) = \varepsilon - \alpha A^2, \qquad \omega(a) = c - bA^2,$$

with $\varepsilon > 0$ and $\alpha > 0$. Using this example the w-equation (7.47) looks as follows (remark that $A^2 = |w|^2$) :

$$\begin{aligned} w_t &= (\lambda + i\omega)w + D\Delta w \\ &= (\varepsilon - \alpha A^2 + i(c - bA^2))w + D\Delta w \\ &= (\varepsilon + ic)w - (\alpha + ib)|w|^2 w + D\Delta w. \end{aligned}$$

Set $w = \hat{w}e^{ict}$ (in some sense, this corresponds to setting $c = 0$), then we get (by $w_t = \hat{w}_t e^{ict} + \hat{w}ice^{ict}$):

$$\begin{aligned} \hat{w}_t e^{ict} + \hat{w}ice^{ict} &= (\varepsilon + ic)\hat{w}e^{ict} + (\alpha + ib)|\hat{w}|^2 \hat{w}e^{ict} + D\Delta\hat{w}e^{ict} \\ \Leftrightarrow \qquad \hat{w}_t &= \varepsilon\hat{w} + (\alpha + ib)|\hat{w}|^2\hat{w} + D\Delta\hat{w}. \end{aligned}$$

Next, we rescale w, t, and r according to

$$\tilde{w} = \left(\frac{\alpha}{\varepsilon}\right)^{1/2} \hat{w}, \qquad \tilde{t} = \varepsilon\hat{t}, \qquad \tilde{r} = \left(\frac{\varepsilon}{D}\right)^{1/2} \hat{r}$$

and get

$$\tilde{w}_t = \tilde{w} - (1 + i\beta)|\tilde{w}|^2\tilde{w} + \Delta\tilde{w}$$

(with $\beta = b/\alpha$).
Indeed, this system (the space-independent version of it, without $\Delta\tilde{w}$) has a limit cycle solution which reads

$$w = \exp(-i\beta t).$$

Interestingly, for larger $|\beta|$ the spiral waves become unstable (in a numerical investigation) and show some chaotic behaviour, see e.g. Fig. 1.23 in [12].

Chapter 8

Pattern formation

Reference: [12, 7]

We already got some ideas about non-homogeneous solutions of reaction-diffusion equations. In this chapter we will deal intensively with possible spatial pattern formation with reaction-diffusion systems. It is not only "nice to see", e.g. how patterns of animal coats can appear, but very essential for life to understand these phenomena, as e.g. morphogenesis (how embryos develop in their early stages) underlies similar processes.

8.1 Turing Mechanisms

We start with Turing's ideas (from 1952): In some situations, it is possible that chemicals react and diffuse in such a ways that the steady state shows heterogeneous spatial patterns of the concentrations. (The concentrations may concern e.g. chemicals or morphogens).
In general, we deal with a problem of the form

$$\frac{\partial c}{\partial t} = f(c) + D\Delta c$$

(c denotes a vector of morphogen concentrations; f as usual the reaction kinetics, D the diffusion coefficients in form of a diagonal matrix). To keep the equations as simple as possible, we usually deal with models for just two chemical species, e.g. A and B, thus the equations read

$$\frac{\partial A}{\partial t} = F(A,B) + D_A\Delta A \tag{8.1}$$
$$\frac{\partial B}{\partial t} = G(A,B) + D_B\Delta B. \tag{8.2}$$

The kinetic terms F and G are always nonlinear in this context.

Turing's idea: Assume that we have a system which tends to a linearly stable state if no diffusion is present. Under certain conditions, a "diffusion driven instability" may evolve, if $D_A \neq D_B$, i.e. spatially inhomogeneous patterns may show up. One species should act as an inhibitor and the other one as an activator.

There are numerous examples for suited kinetics, some typical ones:

Schnakenberg reaction kinetics:

$$\begin{aligned} F(A,B) &= k_1 - k_2 A + k_3 A^2 B \\ G(A,B) &= k_4 - k_3 A^2 B \end{aligned}$$

k_i are positive rate constants. The term k_3A^2B leads to an autocatalytic production of A.

Gierer-Meinhardt:

$$\begin{aligned} F(A,B) &= k_1 - k_2 A + \frac{k_3 A^2}{B} \\ G(A,B) &= k_4 A^2 - k_5 B. \end{aligned}$$

Obviously, A is the activator and B the inhibitor; remark that also here an autocatalytic term is included: $\frac{k_3 A^2}{B}$.

Substrate inhibition system:

$$\begin{aligned} F(A,B) &= k_1 - k_2 A - H(A,B) \\ G(A,B) &= k_3 - k_4 B - H(A,B) \\ H(A,B) &= \frac{k_5 AB}{k_6 + k_7 A + k_8 A^2} \end{aligned}$$

A denotes the concentration of oxygen, B the enzyme uricase. The H-term includes the substrate inhibition via the term $k_8 A^2$. Both H-terms are negative, so they reduce A and B; for large A the rate of reduction is inhibited.

As usual, it is more convenient to analyse the systems in their nondimensional form. All examples considered in this section can be brought into the following form:

$$u_t = \gamma f(u,v) + \Delta u \tag{8.3}$$
$$v_t = \gamma g(u,v) + d\Delta v, \tag{8.4}$$

with $d = D_B/D_A$ (the ratio of the diffusion coefficients). E.g. the reaction terms for the Schnakenberg system read in this form

$$\begin{aligned} f(u,v) &= (a - u + u^2 v) \\ g(u,v) &= b - u^2 v, \end{aligned} \tag{8.5}$$

for the Gierer-Meinhardt system they read

$$\begin{aligned} f(u,v) &= a - bu + \frac{u^2}{v} \\ g(u,v) &= u^2 - v \end{aligned} \tag{8.6}$$

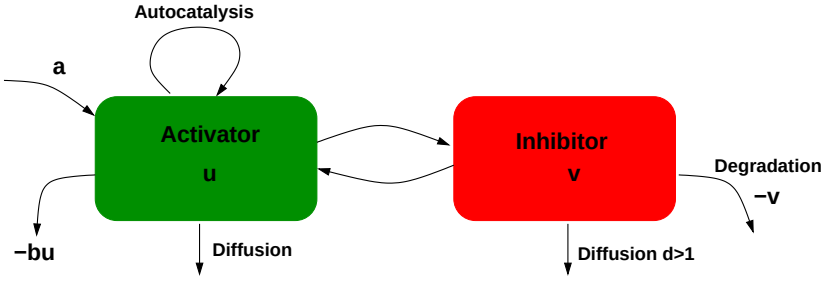
and for the substrate inhibition system

$$\begin{aligned} f(u,v) &= a - u - h(u,v) \\ g(u,v) &= \alpha(b - v) - h(u,v) \\ h(u,v) &= \frac{\rho u v}{1 + u + K u^2}. \end{aligned} \tag{8.7}$$

In this kind of notation, γ can have different meanings:

- $\sqrt{\gamma}$ is proportional to the so-called linear size of the spatial domain in 1D (analogously in 2D proportional to the area of the domain)
- γ is connected to the relative strength of the reaction terms (e.g. increasing γ could represent an activity increase of a rate-limitingstep in the reaction sequence
- an increasing γ could correspond to an decreasing d

Clearly it depends on the present reaction kinetics, and there on the parameter values γ and d if the system can show up a spatial Turing pattern. We will check this later in detail.
The kinetics can be expressed schematically in the following way (as an example for the Gierer Meinhardt activator inhibitor system):



The different diffusion coefficients are important, $d > 1$ corresponds to a local activation in opposite to a long range inhibition (due to the faster diffusion).

8.2 Linear stability analysis for Diffusion-driven instability

The aim of this section is to find necessary and sufficient conditions for the above-mentioned diffusion-driven instability of the homogeneous steady state and how a spatial pattern can be initiated. As usual we need initial conditions (just assumed to be $u(r,0)$, $v(r,0)$) and boundary conditions: We choose zero flux boundary conditions, so patterns are not caused by external input, but by "self-organisation", i.e.

$$(n \cdot \nabla) \begin{pmatrix} u \\ v \end{pmatrix} = 0$$

n denotes the outer normal to ∂B, the closed boundary of the considered domain B.
The considered homogeneous steady state (u_0, v_0) corresponds to the positive solution of

$$f(u,v) = 0, \qquad g(u,v) = 0.$$

Goal is to find a linear instability of this steady state which is only spatially dependent. That means, as already mentioned that the homogeneous steady state must be linearly stable if diffusion (i.e. spatial variation) is absent. The procedure for this is already well-known, the reaction equations (i.e. the spatially homogeneous problem) read

$$u_t = \gamma f(u,v), \qquad v_t = \gamma g(u,v).$$

We use the linearisation at (u_0, v_0): $w = \begin{pmatrix} u - u_0 \\ v - v_0 \end{pmatrix}$, which yields the linear system

$$w_t = \gamma A w, \qquad \text{with } A = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}_{u_0, v_0}$$

and we look for solutions w which are proportional to $e^{\lambda t}$, λ eigenvalue of A. The eigenvalues here can be computed in the standard way

$$\lambda^2 - \gamma(f_u + g_v)\lambda + \gamma^2(f_u g_v)\lambda + \gamma^2(f_u g_v - f_v g_u) = 0 \tag{8.8}$$

and read

$$\lambda_1, \lambda_2 = \frac{\gamma}{2}\left((f_u + g_v) \pm \sqrt{(f_u + g_v)^2 - 4(f_u g_v - f_v g_u)}\right).$$

$Re\lambda < 0$ guarantees stability, i.e.

$$trA = f_u + g_v < 0 \qquad \text{and} \qquad detA = f_u g_v - f_v g_u > 0.$$

Of course, the coordinates of the steady state, (u_0, v_0) depend on the kinetic parameters, so the inequalities for the trace and the determinant imply constraints on the parameters. (Even the plots of isoclines in the phase space can help here!)

In the next step, we use the whole system, including diffusion. Linearisation at the steady state (u_0, v_0) or in the w-coordinates $w = 0$ looks as follows:

$$w_t = \gamma A w + D\Delta w, \qquad \text{with } D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}. \tag{8.9}$$

As a first step, we consider the time-independent solution $W(r)$ of the spatial eigenvalue problem

$$\begin{aligned} \Delta W + k^2 W &= 0 \\ (n \cdot \nabla) W &= 0 \qquad \text{for } r \text{ on } \partial B \qquad \text{(boundary conditions)} \end{aligned}$$

k is the eigenvalue. For the 1D case (e.g. $0 \le x \le \alpha$) the eigenfunctions $W = \cos(n\pi x/a)$ (n integer) satisfy the zero flux conditions at $x = 0$ and $x = a$; the corresponding eigenvalues are $k = n\pi/a$. In this context, k is called the wavenumber, vice versa $\frac{1}{k} = \frac{a}{n\pi}$ is a measure of the wavelike pattern (and proportional to the wavelength $\omega = \frac{2\pi}{k} = \frac{2a}{n}$. As long as we deal with finite domains, there is a discrete set of possible wavenumbers.
So, let $W_k(r)$ denote the eigenfunction which belongs to wavenumber k (it satisfies the zero flux boundary condition!). We deal with a linear problem, so the solutions $w(r,t)$ of (8.9) can be displayed as

$$w(r,t) = \sum_k c_k e^{\lambda t} W_k(r),$$

here, the constants c_k can be determined by a Fourier expansion of the initial condition in terms of the time-independent solutions $W_k(r)$. Remark that λ denotes the eigenvalue for the temporal growth (not to mix it up with the "spatial eigenvalue problem")!
We take this approach and insert it into (8.9) and take into account the properties of W_k and get for each k:

$$\begin{aligned} \lambda W_k &= \gamma A W_k + D\Delta W_k \\ &= \gamma A W_k - Dk^2 W_k. \end{aligned}$$

(The term $e^{\lambda t}$ appears in each term and can thus be cancelled out). W_k are required to be nontrivial solutions, thus we determine λ as roots of the characteristic polynomial

$$det(\lambda I - \gamma A + Dk^2) = 0.$$

Using the definitions of the matrices A and D from above, this corresponds to

$$\lambda^2 + \lambda[k^2(1+d) - \gamma(f_u + g_v)] + h(k^2) = 0, \tag{8.10}$$

where

$$h(k^2) = dk^4 - \gamma(df_u + g_v)k^2 + \gamma^2 detA.$$

As usual, the steady state (u_0, v_0) is (linearly) stable if $Re\lambda < 0$ for both eigenvalues λ.
Remark that we wanted to have a stable steady state in case of absent spatial effects, which corresponds to $Re\lambda(k^2 = 0) < 0$, which again corresponds to (8.8) and leads to the conditions for the trace and the determinant above. Second, we require $Re\lambda(k) > 0$ for a $k \neq 0$, i.e. such that the steady state is unstable if spatial disturbances (i.e. the diffusion) are present. There are two possibilities for this: Either $k^2(1+d) - \gamma(f_u + g_v)$ is negative (which corresponds to the coefficient of λ in (8.10)) or $h(k^2) < 0$ for some $k \neq 0$. From the trace condition (for the case without diffusion) we have $(f_u + g_v) < 0$, and $k^2(1+d) > 0$ for all $k \neq 0$ (generally true), thus we find

$$(k^2(1+d) - \gamma(f_u + g_v)) > 0,$$

thus the coefficient for λ is always positive. The only remaining possibility for $Re\lambda(k^2)$ is hence $h(k^2) < 0$ for some k.
It is useful to consider the explicit formula for λ (solution of (8.10)):

$$2\lambda = -(k^2(1+d) - \gamma(f_u + g_v)) \pm \sqrt{(k^2(1+d) - \gamma(f_u + g_v))^2 - 4h(k^2)}.$$

h was defined as $h(k^2) = dk^4 - \gamma(df_u + g_v)k^2 + \gamma^2 detA$. The determinant of A was needed to be positive (for the stability of the non-spatial problem), so we need $(df_u + g_v) > 0$. From the trace condition $(f_u + g_v < 0)$ it implies that $d \neq 1$ and f_u and g_v need opposite signs to allow for this condition.
Short excurs to the kinetics of the Schnakenberg system: the stationary state for the kinetics can be easily computed via

$$f(u_0, v_0) = a - u_0 + u_0^2 v_0 = 0 \qquad \text{and} \qquad g(u_0, v_0) = b - u_0^2 v_0 = 0$$

to be

$$u_0 = b + a, \qquad v_0 = \frac{b}{(a+b)^2}$$

where $b > 0$ and $a + b > 0$. Hence, we find at the stationary point:

$$\begin{aligned} f_u|_{(u_0,v_0)} &= -1 + 2u_0 v_0 = -1 + 2(b+a) \cdot \frac{b}{(a+b)^2} = \frac{b-a}{a+b} \\ g_v &= -u_0^2 = -(b+a)^2 < 0 \end{aligned}$$

For the linear stability of the non-diffusive model, we claimed that $f_u + g_v < 0$, so in this case we have $f_u > 0$. In order to allow for $df_u + g_v > 0$, then we need $d > 1$. What does this mean? The diffusion of the inhibitor must be faster than the diffusion of the activator!

Still we have not found a sufficient condition for $Re\lambda > 0$ (only a necessary condition). In order to get a negative $h(k^2)$ for some k, the minimum h_{min} must be negative. Setting the first derivative of h to 0,

$$h' = 2dk^2 - \gamma(df_u + g_v) = 0 \qquad \Leftrightarrow \qquad k^2 = k_m^2 = \frac{\gamma(df_u + g_v)}{2d}$$

yields

$$\begin{aligned} h_{min} &= d\left(\frac{\gamma(df_u+g_v)}{2d}\right)^2 - \gamma(df_u+g_v)\frac{\gamma(df_u+g_v)}{2d} + \gamma^2 det(A) \\ &= \gamma^2\left[det(A) - \frac{(df_u+g_v)}{4d}\right] \end{aligned}$$

So, as we want to have a $k^2 \neq 0$ with $h(k^2) < 0$, the necessary condition reads

$$det(A) < \frac{(df_u+g_v)^2}{4d}.$$

The system changes its behaviour when $h_{min} = 0$, hence there we have the equality $det(A) = \frac{(df_u+g_v)^2}{4d}$. If all kinetic parameters are fixed, we can define a critical diffusion coefficient ratio $d_c > 1$ as the appropriate root of this equation:

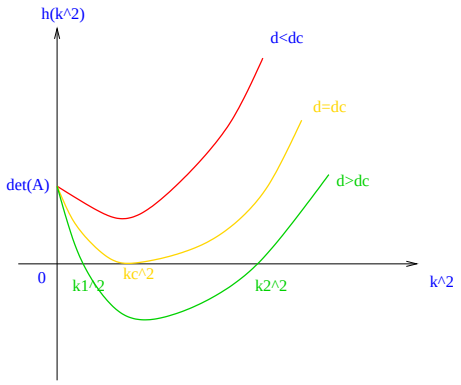
$$\frac{d_c^2 f_u^2 + 2d_c f_u g_v + g_v^2}{d_c} - 4\underbrace{(f_u g_v + f_v g_u)}_{det(A)} = 0 \qquad \Leftrightarrow \qquad d_c^2 f_u^2 + 2(2f_v g_u - f_u g_v)d_c + g_v^2 = 0,$$

Correspondingly, we can determine the critical wavenumber k_c by

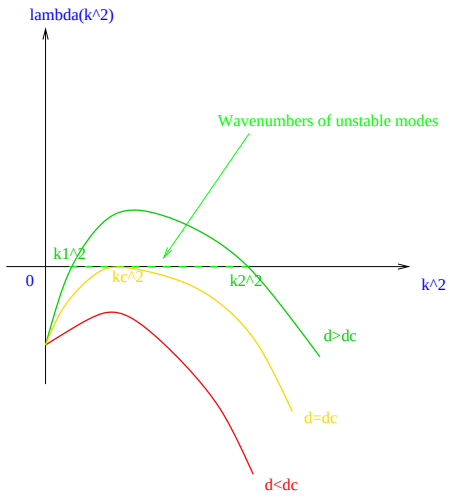
$$k_c^2 = \gamma\frac{d_c f_u + g_v}{2d_c} = \gamma\sqrt{\frac{det(A)}{d_c}} = \gamma\sqrt{\frac{f_u g_v - f_v g_u}{d_c}}.$$

In case of $h(k^2) < 0$, there are two zeros k_1^2 and k_2^2 of $h(k^2) = 0$, and the unstable wavenumbers are between them, $k_1^2 < k^2 < k_2^2$, i.e.

$$\begin{aligned} k_1^2 &= \frac{\gamma}{2d}\left[(df_u+g_v) - \{(df_u+g_v)^2 - 4ddet(A)\}^{1/2}\right] < k^2 \\ &< \frac{\gamma}{2d}\left[(df_u+g_v) + \{(df_u+g_v)^2 - 4ddet(A)\}^{1/2}\right] = k_2^2. \end{aligned}$$



Vice versa, one can plot (the largest) $\lambda(k^2)$ against k_2 (the so-called dispersion relation). Of course, in the unstable range, we have $Re\lambda(k^2) > 0$.



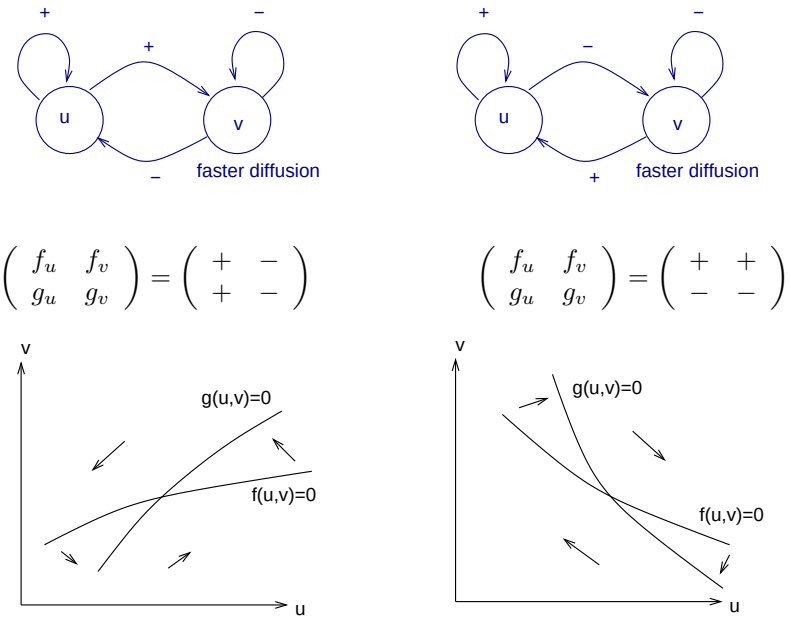
Obviously, if $d > d_c$ there is a maximum for $Re\lambda(k^2) > 0$ for a wavenumber k_m, it is exactly the one from above. Thus, a fastest growing mode in $w = \int_k c_k e^{\lambda t} W_k(r)$ exists.
Furthermore, only those modes with $Re\lambda(k^2) > 0$ are relevant for increasing t, as all other modes tend to zero exponentially. So, using the above introduced range $k_1^2 < k^2 < k_2^2$, there $h(k^2) < 0$ and subsequently $Re\lambda(k^2) > 0$, we find

$$w(r,t) \sim \sum_{k_1}^{k_2} c_k e^{\lambda(k^2)t} W_k(r) \qquad \text{for large } t.$$

Remark: The wavenumbers are discrete when considering a finite domain, so only certain k values may be in the relevant range.
Hence, we need the following conditions satisfied in general (to allow for the desired instability behaviour):

$$\begin{aligned} f_u + g_v &< 0 \\ f_u g_v - f_v g_u &> 0 \\ d f_u + g_v &> 0 \\ (d f_u + g_v)^2 - 4d(f_u g_v - f_v g_u) &> 0. \end{aligned}$$

(first condition: $trA < 0$, second condition: $detA > 0$, forth condition: then $h_{min} < 0$) In general, two typical cases of diffusion driven instability are possible:



Left case: u is the activator of v (and self-activating), v is the inhibitor (self-inhibition and inhibition of u). For the pattern formation, the inhibitor must diffuse faster than the activator.
Right case: v is the activator of u (but self-inhibiting), diffuses faster. u inhibits v (but is self-activator).

8.3 Analysis of Pattern Initiation for the Schnakenberg system

Reference: [12]

Here we consider the Schnakenberg system including diffusion, as introduced above (in the simplified version):

$$u_t = \gamma f(u,v) + u_{xx} = \gamma(a - u + u^2 v) + u_{xx} \tag{8.11}$$
$$v_t = \gamma g(u,v) + d v_{xx} = \gamma(b - u^2 v) + d v_{xx} \tag{8.12}$$

We recollect the most important results from the analyses above:

- Positive stationary state $(u_0, v_0) = (a+b, \frac{b}{(a+b)^2})$ with $b > 0$ and $a + b > 0$

- Partial derivatives at the stationary state:

$$\begin{aligned} f_u &= \frac{b-a}{a+b} \\ f_v &= (a+b)^2 > 0 \\ g_u &= -\frac{2b}{a+b} < 0 \\ g_v &= -(a+b)^2 < 0, \end{aligned}$$

  furthermore $f_u g_v - f_v g_u = (a+b)^2 > 0$.

- f_u and g_v must have opposite signs $\rightsquigarrow b > a$ is required.

Now we can check the above mentioned criteria for allowing the instability behaviour, how they look in our special case:

$$\begin{aligned} f_u + g_v < 0 &\Rightarrow 0 < b-a < (a+b)^3 \\ f_u g_v - f_v g_u > 0 &\Rightarrow (a+b)^2 > 0 \\ df_u + g_v > 0 &\Rightarrow d(b-a) > (a+b)^3 \\ (df_u + g_v)^2 - 4d(f_u g_v - f_v g_u) > 0 &\Rightarrow (d(b-a) - (a+b)^3)^2 > 4d(a+b)^4 \end{aligned}$$

By this, a domain in the (a, b, d) parameter space is defined, which is called the "pattern formation space" or "Turing space".

We consider the 1D situation on a finite interval $[0, p]$, so our problem in form of the corresponding eigenvalue problem reads

$$W_{xx} + k^2 W = 0, \qquad W_x = 0 \text{ for } x = 0, p. \tag{8.13}$$

The solutions of (8.13) read

$$W_n(x) = A_n \cos(n\pi x/p), \qquad n = \pm 1, \pm 2, \ldots,$$

A_n are constants which can be chosen arbitrarily, and the eigenvalues $k = n\pi/p$ are discrete wavenumbers. The unstable modes can be found in the following range:

$$\gamma L(a,b,d) = k_1^2 < k^2 = \left(\frac{n\pi}{p}\right)^2 < k_2^2 = \gamma M(a,b,d),$$

where

$$L = \frac{[d(b-a) - (a+b)^3] - \{[d(b-a) - (a+b)^3]^2 - 4d(a+b)^4\}^{1/2}}{2d(a+b)} \tag{8.14}$$

$$M = \frac{[d(b-a) - (a+b)^3] + \{[d(b-a) - (a+b)^3]^2 - 4d(a+b)^4\}^{1/2}}{2d(a+b)}. \tag{8.15}$$

one can formulate this idea also in terms of the wavelength $\omega = \frac{2\pi}{k}$, there the range of unstable models W_n includes wavelengths which are bounded by ω_1 and ω_2 in the following way:

$$\frac{4\pi^2}{\gamma L(a,b,d)} = \omega_1^2 > \omega^2 = \left(\frac{2p}{n}\right)^2 > \omega_2^2 = \frac{4\pi^2}{\gamma M(a,b,d)}. \tag{8.16}$$

Remark: the scale γ plays an important role, since a sufficiently small γ prevents that an allowable k (or vice versa an allowable ω can be found in the range for fixed parameters a, b and d).
Taken together, the resulting spatially heterogeneous solution consists of the unstable modes, i.e.

$$w(x,t) \sim \sum_{n_1}^{n_2} C_n \exp\left[\lambda\left(\frac{n^2\pi^2}{p^2}\right)t\right] \cos\frac{n\pi x}{p}.$$

λ is the positive root of

$$\lambda^2 + \lambda(k^2(1+d) - \gamma(f_u + g_v)) + h(k^2) = 0,$$

n_1 is defined as the smallest integer $\geq \frac{pk_1}{\pi}$, correspondingly n_2 is the largest integer $\leq \frac{pk_2}{\pi}$. The coefficients C_n (which are constants) are determined by the initial conditions for w and its Fourier series. (Remark that in biological reality, all Fourier modes may appear, as a certain stochasticity is always included).

How to generalise this approach for the 2D situation? We consider a rectangular domain $B = (0,p)\times(0,q)$, then the spatial eigenvalue problem reads

$$\Delta W + k^2 W = 0 \qquad \text{for } (x,y) \in B \tag{8.17}$$
$$(n \cdot \nabla) W = \qquad \text{for } (x,y) \text{ on } \partial B \tag{8.18}$$

in this case the eigenfunctions read

$$W_{p,q}(x,y) = C_{n,m} \cos\frac{n\pi x}{p} \cos\frac{m\pi y}{q}, \qquad \text{with} k^2 = \pi^2 \left(\frac{n^2}{p^2} + \frac{m^2}{q^2}\right).$$

(n and m are integers, of course). All approaches of the 1D case can be transferred to the 2D case, we just have to replace the wavenumber by the correct one for the 2D case, i.e. $k^2 = \pi^2 \left(\frac{n^2}{p^2} + \frac{m^2}{q^2}\right)$. Hence, the 2D modes with n, m such that the corresponding k lies within the "unstable range" again are linearly unstable. This means: The unstable spatially patterned solution can be written as

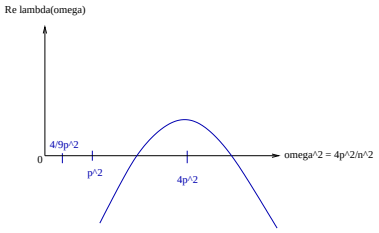
$$w(x,y,t) \sim \sum_{n,m} C_{n,m} e^{\lambda(k^2)t} \cos\frac{n\pi x}{p} \cos\frac{m\pi y}{q}$$

with

$$\gamma L(a,b,d) = k_1^2 < k^2 = \pi^2 \left(\frac{n^2}{p^2} + \frac{m^2}{q^2}\right) < k_2^2 = \gamma M(a,b,d).$$

It is sufficient to take the sum over those pairs (n,m) which satisfy this inequality.

Next question: How does such a pattern look like? (We restrict ourselves to the 1D case again)
We assume a situation where γ measures the domain size, and there is only the wavenumber for $n = 1$ which lies inside the range of unstable wavenumbers. The corresponding typical dispersion relation for $Re\lambda$ (as growth factor) dependent on the wavelength ω looks as follows:



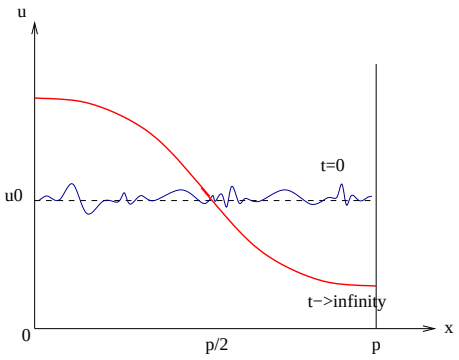
Obviously, there is only one unstable mode then: $\cos(\pi x/p)$ and the growing instability reads

$$w(x,t) \sim C_1 \exp\left[\lambda\left(\frac{\pi^2}{p^2}\right)t\right] \cos\frac{\pi x}{p}$$

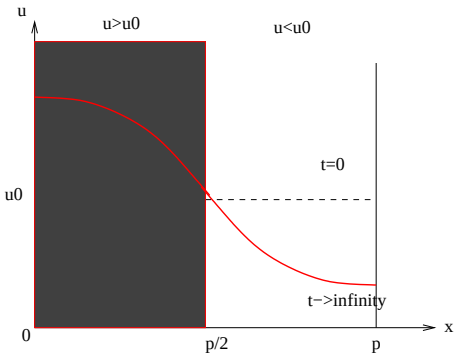
(λ as usual; $k^2 = (\pi/p)^2$). All other modes are stable, i.e. decay exponentially in time.
Remember that w was a vector in our approach, including the two components for u and v. For a better understanding of the consequences of this result, we choose $C_1 = \begin{pmatrix} \varepsilon \\ \varepsilon \end{pmatrix}$ (instead of determining it from given initial conditions), where $\varepsilon > 0$ small. Then u can be written as

$$u(x,t) \sim u_0 + \varepsilon \exp\left[\lambda\left(\frac{\pi^2}{p^2}\right)t\right] \cos\frac{\pi x}{p}.$$

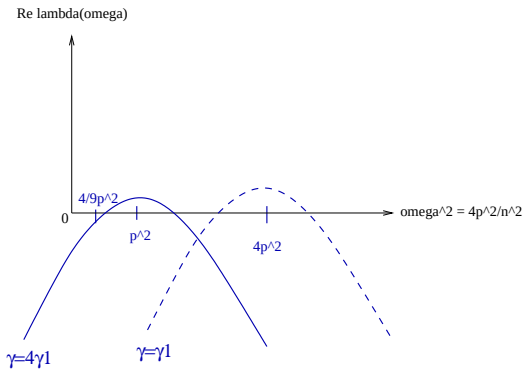
Now, the (only) unstable mode is dominating for an increasing t. The typical pattern looks as follows:



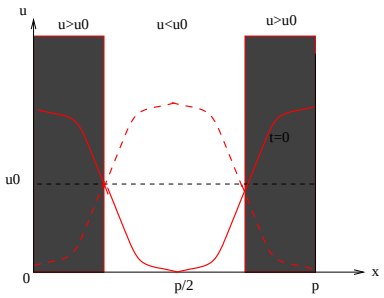
Of course, if this exponentially growing solution is be present for all times $t \to \infty$, it would correspond to $u \to \infty$ for $t \to \infty$. But this behaviour is only realistic not too far away from the homogeneous steady state, as it was derived from the linear approximation. For the real system, the kinetics bounds the solution to a confined set within the positive quadrant. Nevertheless, one assumes that the growing solution looks somehow similar to the spatial pattern which was derived for the single cosinus mode.
A short remark concerning the representation of the spatial patterns: In principle, one has continuously varying concentrations. For showing the main behaviours, one just distinguishes between regions, where the concentration is below (non-coloured) respectively above (coloured) a certain threshold. For the threshold, the usual method is to choose the state state value u_0. In our example, the pattern hence looks as follows:



In the next step, we consider the size-dependency. We assume that γ represents somehow the domain size, e.g. concretely as scale of one space dimension; i.e. doubling of the domain size would correspond to increasing γ by a factor of 4. For the dispersion relation this means that it is shifted such that the wavelength of the unstable mode is now located at $\omega = p$, which corresponds to $n = 2$:



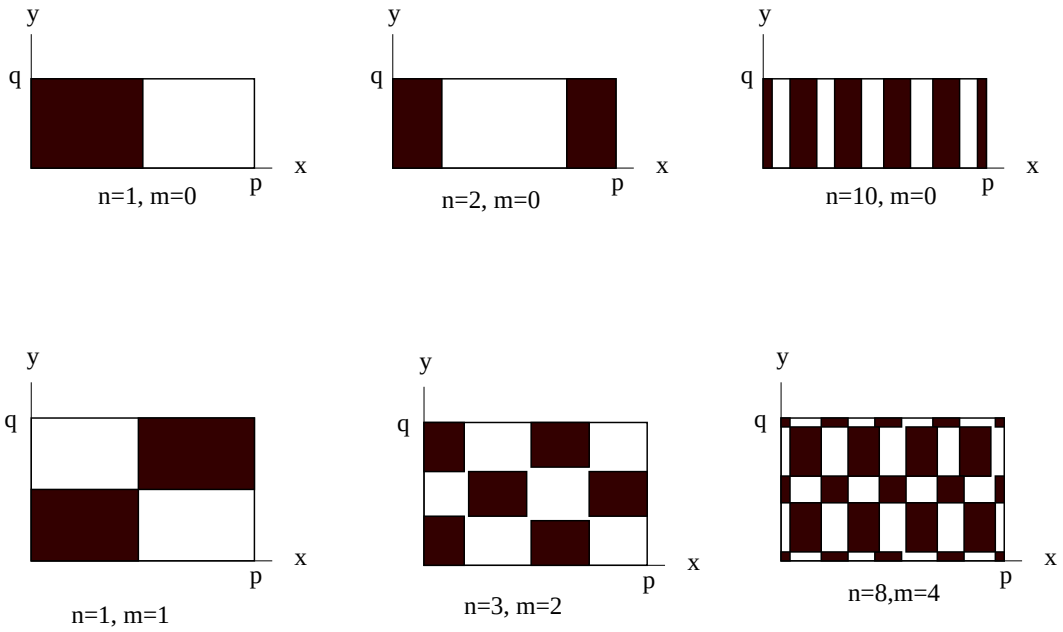
Then, the corresponding solution / spatial pattern looks as follows:



Remark that also the "$-cos$" solution could appear (shown by the dashed line), which would yield the "mirror image". Which one appears in reality depends on the initial conditions.

In the same way, we can find: The larger the domain is (included into the model by increasing γ), the higher the mode which is unstable, yielding a higher number of stripes in the pattern.
In the other direction, if γ is chosen too small, i.e. then the mode $n = 1$ is not unstable (due to the parabola $Re\lambda(\omega)$ is not positive for $\omega = 4p^2/n^2$, $n = 1$), then no mode is unstable and no spatial pattern can appear. We call this the concept of a critical domain size. Especially for developmental biology, this is an important fact - too small domains do not allow for patterns!

These ideas can also be transferred to the 2D problem. Big difference here: A given scale represents the scale, but there is a domain geometry which consists of length p and width q. Hence, different modes may be unstable for length respectively width. Some examples for typical (temporally growing) 2D spatial patterns:



Generalising this approach to more complicated 2D domains is not that easy. For that, we need to solve the eigenvalue problem of type

$$\Delta\psi + k^2\psi = 0, \qquad (n \cdot \nabla)\psi) = 0 \quad \text{for } r \text{ on } \partial B.$$

The only chance to do so (even for circular domains) is to try to compute the eigenvalues numerically. One approach uses a kind of tessellation of the plane by symmetric domains (for some symmetric domains, elementary solutions can be determined; e.g. for squares, hexagons, rhombi and triangles).

Heterogeneity function

Starting with the typical mechanism,

$$\begin{aligned} u_t &= \Delta u + \gamma f(u,v) \\ v_t &= d\Delta v + \gamma g(u,v), \end{aligned}$$

in 1D (space), we assume that it is diffusionally unstable; the solutions are assumed to tend to steady state solutions $U(x)$ and $V(x)$ for $t \to \infty$ (i.e. spatially inhomogeneous). The domain size is again expressed by using the parameter γ, so we can assume the space variable to be normalised in such a way that $x \in (0,1)$. Such a solution $U, V)$ thus satisfies the following (dimensionless) equations:

$$\begin{aligned} U'' + \gamma f(U,V) &= 0 \\ dV'' + \gamma g(U,V) &= 0 \end{aligned}$$

with the boundary conditions (homogeneous Neumann)

$$U'(0) = U'(1) = V'(0) = V'(1) = 0.$$

Now, the heterogeneity function can be defined by

$$H = \int_0^1 (U'^2 + V'^2)\, dx \geq 0.$$

Obviously, H is nonnegative and only depends on the system parameters and γ. Integration by parts yields (applying the boundary conditions):

$$H = \underbrace{[UU' + VV']_0^1}_{=0} - \int_0^1 (UU'' + VV'')\, dx$$

In this equation, we can replace U'' and V'' by the corresponding terms from above, i.e.

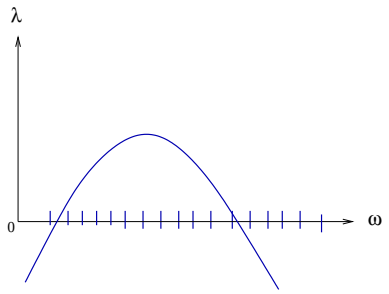
$$H = \frac{\gamma}{d} \int_0^1 (dU f(U,V) + V g(U,V))\, dx.$$

Already from the definition is is clear that if there is no spatial patterning, we get $H = 0$; then U and V correspond to the uniform steady state solutions of $f(U,V) = g(U,V) = 0$.

8.4 Mode Selection

Reference: [12]

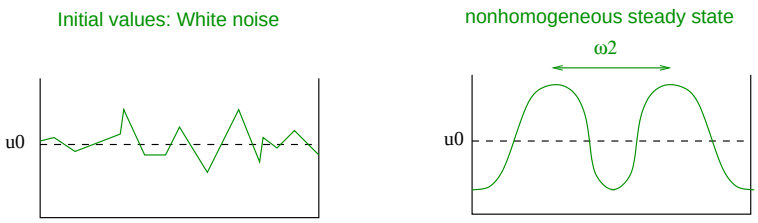
Until now, we allowed only for one unstable mode, where the developing pattern was more or less "fixed" then. In general, several wavenumbers may be linearly unstable. We consider a situation with a finite domain, so the spectrum of the eigenvalues is discrete. The typical situation for the basic dispersion relation then looks as follows:



Question: Which pattern does appear in reality? There are several possibilities, e.g. dependent on the initial conditions!

8.4.1 White noise

Here, one assumes that an initial perturbation contains all modes (when expanded in terms of the eigenfunctions). Hence, all unstable modes are stimulated; the one with the maximum λ (denoted by ω_2) will be the dominating mode, it has the fastest growth. So the inhomogeneous steady state may show up with wavelength ω_2.



8.4.2 Travelling wave initiation of patterns

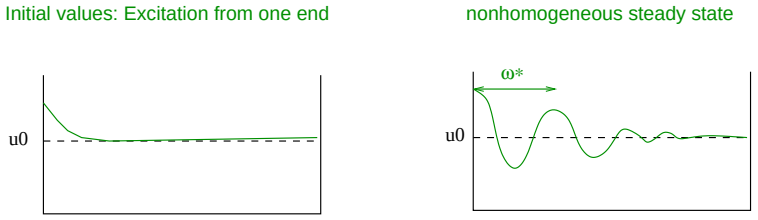
Here, we start with an initial disturbance at one end of the domain. One expects a final pattern with a wavelength which is inside the unstable band (refer to the dispersion relation).
We start with a general survey, how the wavenumber can be calculated. For that, we consider with an infinite 1D domain, in this case a general linear system can be written as

$$\mathcal{J}w = 0, \qquad w(x,t) \sim \exp(ikx + \lambda t), \tag{8.19}$$

λ as function of k, i.e. $\lambda = \lambda(k)$, $\mathcal{J}w$ is assumed to be a linear operator which is associated with the linear form of reaction diffusion equations. (E.g., one can have in mind $\mathcal{J} = (\partial/\partial t) - \gamma A - D\Delta$) and a typical dispersion relation $\lambda(k)$.
The general solution of (8.19) reads

$$w(x,t) = \int A(k) \exp(ikx + \lambda(k)t)\, dk,$$

where $A(k)$ is determined by the initial conditions $w(x,0)$ and the consequent Fourier transform.
We assume that the initial conditions $w(x,0)$ are restricted to a small finite domain around $x = 0$ and from there, the pattern starts to propagate. We are interested in a "wavelike" pattern generation which looks somehow in the following way:



As we look for such a wavelike solution, the form of the solution with some distance from the origin is of interest, especially the asymptotic form of the solutions for large x and t, but in such a way that x/t is $\mathcal{O}(1)$ due to the velocity $c = x/t$ and we can follow in some sense the wave front. The solution can be rewritten as

$$w(x,t) = \int A(k) \exp(\sigma(k)t)\, dk, \qquad \text{with } \sigma(k) = ikc + \lambda(k) \text{ and } c = x/t.$$

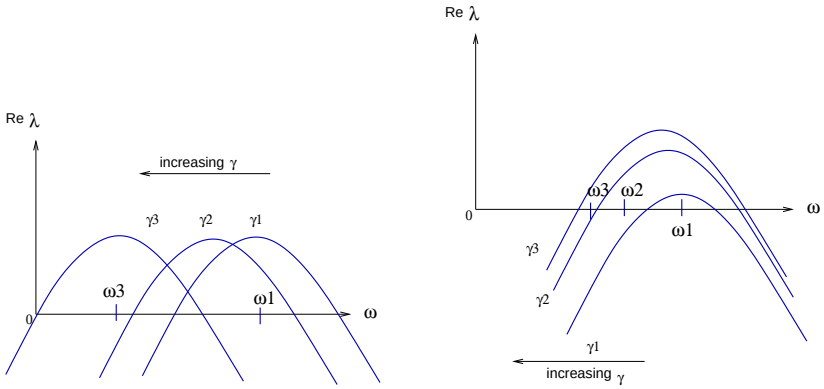
By using the so-called "method of steepest descents" (we do not consider it here in detail), one can find the asymptotic form of the solution:

$$w(x,t) \sim \frac{K}{t^{1/2}} \exp\left(t(ick_o + \lambda(k_0))\right),$$

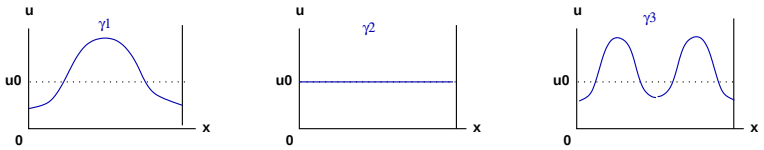
with K constant and (the complex) k_0 is determined by $\sigma'(k_0) = ic + \lambda'(k_0) = 0$.

8.4.3 Pattern formation in growing domains

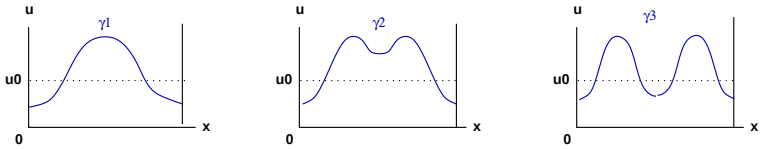
Problem: If the relevant domain grows, this may affect γ and by that the dispersion curve will move. For a growing γ this may lead to the following shifts:



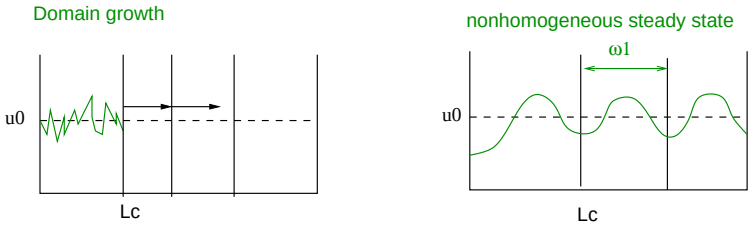
Left situation: For $\gamma = \gamma_1$ wavelength ω_1 corresponds to the mode which is excited and starts to grow. For an increasing domain (i.e. growing γ), for $\gamma = \gamma_2$ there is no mode at all in the unstable waveband, so the solution must tend to the spatially uniform steady state; the pattern decays. For further increasing γ, i.e. $\gamma = \gamma_2$ the next unstable mode for ω_3 appears with a pattern.
This means: The pattern formation is in some sense a discrete process; for an increasing γ with more structure, but can be in such a way that there are regimes of spatial homogeneity are present.



Right situation: In this case, the increasing γ just increases the band of unstable modes, so unstable modes stay unstable all the time, but the dominant mode may change (e.g. from ω_1 to ω_3). This yields a more "continuous" switch from one mode to another, which looks in the following way:



These typical types of "bifurcations" are also very relevant in Morphogenesis, e.g. for the formation of the limbs. Dependent on how the influence of the parameters is (as shown above), a Y-shaped bone may develop, either with a region of homogeneity in between (so two separate bones develop) or just in one piece. For some pictures, see e.g. in Murray [12] Section 6.6. Possibly, the pattern formation on a growing domain works in such a way that the first unstable mode which can be excited, denoted by ω_1, stays dominant, then the following pattern may evolve:



8.5 Nonexistence of spatial patterns in reaction diffusion systems

Reference: [12] Recall the (spatially) 1D scalar reaction diffusion system of the form

$$\begin{aligned} u_t &= f(u) + u_{xx}, \qquad x \in (0,1), \ t > 0 \\ u_x(0,t) &= u_x(1,t) = 0, \qquad t > 0. \end{aligned}$$

Let $u = u_0$ be the stable steady state solution of $f(u) = 0$, then, the only stable solution will be the spatially homogeneous on $u = u_0$. Of course, if there are several stable solutions, it depends on the

initial conditions, which one will be assumed. In the 1D case (spatial dimension) one can show that any spatially nonhomogeneous steady state solution is unstable.
In higher spatial dimensions this mustn't be true, when $f(u)$ has two linearly stable steady states. A pattern may evolve, it depends on the specific domain boundaries (e.g. nonconvex boundaries), how much "transport" is possible from one steady state to another an so on.

In this section, we consider shortly the case of large diffusion. Of course, for the pattern formation it was necessary to have different diffusion coefficients for different reactants in the reaction diffusion system. But what happens is the diffusion becomes very large? Will it destroy patterns?

We start with a two-species system:

$$u_t = f(u,v) + D_1 u_{xx} \tag{8.20}$$
$$v_t = g(u,v) + D_2 v_{xx} \tag{8.21}$$

and assume homogeneous Neumann boundary conditions and initial conditions as follows:

$$\begin{aligned} u_x(0,t) &= u_x(1,t) = v_x(0,t) = v_x(1,t) = 0 \\ u(x,0) &= u_0(x) \\ v(x,0) &= v_0(x). \end{aligned}$$

For compatibility of the initial and the boundary conditions, we claim that $u_0'(x) = v_0'(x) = 0$ on $x = 0, 1$.
Next, a so-called energy integral E is defined as follows:

$$E(t) = \frac{1}{2}\int_0^1 (u_x^2 + v_x^2)\, dx.$$

(Remark that this corresponds exactly to the heterogeneity function, except for the factor $\frac{1}{2}$.)
The t-derivative reads

$$\frac{dE}{dt} = \int_0^1 (u_x u_{xt} + v_x v_{xt})\, dx$$

We can take (8.20) and (8.21), derive it with respect to x and insert it into this equation (use partial integration and the zero flux boundary conditions):

$$\begin{aligned} \frac{dE}{dt} &= \int_0^1 [u_x(D_1 u_{xx})_x + u_x(f_u u_x + f_v v_x) + v_x(D_2 v_{xx})_x + v_x(g_u u_x + g_v v_x)]\, dx \\ &= \underbrace{[u_x D_1 u_{xx} + v_x D_2 v_{xx}]_0^1}_{=0} - \int_0^1 (D_1 u_{xx}^2 + D_2 v_{xx}^2)\, dx \\ &\quad + \int_0^1 \left[f_u u_X^2 + g_v v_x^2 + (f_v + g_u) u_x v_x\right]\, dx. \end{aligned}$$

For simplification of the notation, we introduce

$$d = \min(D_1, D_2), \qquad m = \max_{u,v} \left(f_u^2 + f_v^2 + g_u^2 + g_v^2\right)^{(1/2)},$$

the $\max_{u,v}$ means that all possible solution values for u and v are taken and the maximum is determined over these. Hence we can formulate the following estimate (remember the Poincare inequality: $\int_0^1 u_{xx}^2\, dx \geq \pi^2 \int_0^1 u_X^2\, dx$):

$$\begin{aligned} \frac{dE}{dt} &\leq -d\int_0^1 (u_{xx}^2 + v_{xx}^2)\, dx + 4m\int_0^1 (u_x^2 + v_X^2)\, dx \\ &\leq (4m - 2\pi^2 d)E \end{aligned}$$

This estimation has to be considered carefully: If d is so large that $(4m - 2\pi^2 d) < 0$, then we obviously get $\frac{dE}{dt} < 0$ and consequently $E \to 0$ for $t \to \infty$ (by definition it is $E(t) \geq 0$). But, having in mind the definition of E, this implies that $u_x \to 0$ and $v_x \to 0$ which means spatial homogeneity in the solution.
Remark that this is just an example, no "if and only if situation", we have used estimations which can be chosen differently.

This idea can be transferred to general reaction diffusion systems of the form

$$u_t = f(u) + D\Delta u$$

(u vector with components u_i, $i = 1, 2, \ldots, n$, D diagonal matrix with coefficients $D_i > 0$, $i = 1, 2, \ldots, n$), initial conditions

$$u(r, 0) = u_0(r)$$

and homogeneous Neumann boundary conditions

$$(n \cdot \nabla)u = 0$$

(Assume that the reaction kinetics guarantees that all solutions u stay bounded for all $t \geq 0$).
In this general case, the energy $E(t)$ is defined by

$$E(t) = \frac{1}{2} \int_B \|\nabla u\|^2 \, dr \qquad (\text{with } \|nablau\|^2 = \sum_{i=1}^{n} |\nabla u_i|^2).$$

Let $d := \min\{D_i, i = 1, 2, \ldots, n\}$ the smallest diffusion coefficient and

$$m = \max_u \|\nabla_u f(u)\|$$

where u means the maximum for all possible solution values for u (similar to above) and ∇_u denotes the gradient operator with respect to u.
Again, we need to differentiate $E(t)$, here we use the scalar product (notation $\langle a, b \rangle$):

$$\begin{aligned}
\frac{dE}{dt} &= \int_B \langle \nabla u, \nabla u_t \rangle \, dr \\
&= \int_B \langle \nabla u, \nabla D\Delta u \rangle \, dr + \int_B \langle \nabla u, \nabla f \rangle \, dr \\
&= \underbrace{\int_{\partial B} \langle \nabla u, D\Delta u \rangle \, dr}_{=0} - \int_B \langle \Delta u, D\Delta u \rangle \, dr + \int_B \langle \nabla u, \nabla_u f \cdot \nabla u \rangle \, dr \\
&\leq -d \int_B |\Delta u|^2 \, dr + mE.
\end{aligned}$$

(again using "partial integration" with the boundary conditions). Next we need the analogue to the Poincare inequality. Even this can be transferred and reads in general

$$\int_B |\Delta u|^2 \, dr \geq \mu \int_B \|\nabla u\|^2 \, dr,$$

there μ is the least positive eigenvalue of the eigenvalue problem

$$\Delta\phi + \mu\phi = 0, \qquad (n \cdot \nabla)\phi = 0(\text{on } \partial B$$

(for ϕ a scalar). Inserting this above, we get

$$\frac{dE}{dt} \leq (m - 2\mu d)E$$

and hence

$$\lim_{t \to \infty} E(t) = 0 \qquad \text{if } m < 2\mu d.$$

This means again: If the smallest diffusion coefficient is "large enough", then we get $\nabla u \to 0$ which corresponds to a homogeneous solution, all spatial patterns disappear for $t \to \infty$.

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